

Plenary Lecture : **PLEN-1**

Plenary Lecture

Room 211, THU 13:30

Chair: Seokhee Kim (Seoul National University)

Molecular Machines that Make Membranes

Daniel Kahne

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

The Kahne Lab is interested in understanding the biogenesis of the cell envelope of Gram-negative bacteria, in particular peptidoglycan biosynthesis and outer membrane assembly. The assembly of this membrane must be accomplished outside the cell in the absence of an obvious energy source. My research focuses on identifying and understanding the machinery necessary for proper assembly of this membrane barrier, as well as the mechanisms that lead to defects. Because the outer membrane creates an effective permeability barrier to most antibiotics, understanding how to interfere with its assembly could provide new targets for antibiotic discovery.

Award Lecture : **AWARD-1**

Award Lecture

Room 325A+B, FRI 13:30

Chair: Yung Doug Suh (KRICT)

Taikyue Ree: Tracing the Work of a Leading Chemist of His Time from a Modern Perspective

Seong Keun Kim

Department of Chemistry, Seoul National University, Korea

This award lecture aims to shed light on the work of the namesake of the award, Prof. Taikyue Ree, from the perspective of modern chemistry. Prof. Ree's doctoral work on the catalytic reaction of CO is recounted with some examples of modern surface chemistry. His first paper published in the United States was on the calculation of the dipole moments of some substituted benzenes, which may likely be the first attempt to calculate the distribution of electrostatic charge within a molecule. Modern examples of anomalous electrostatic charge distribution will be presented, along with an experimental attempt to verify such charge distribution when the charge is "divided" in a molecule. The role of electrostatic charge in stabilizing an otherwise unstable structure of a simple molecule such as CO₂ is to be presented as well. Another of his early paper on the mechanism of reaction between alkali metals and hydrogen will also be viewed from the context of molecular reaction dynamics developed some 20 years later. The lecture will note some anecdotal incidents drawn from literature and also from personal encounters.

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-1**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 15:40

Chair: Changjin Lee (KRICT)

Recollecting the Early History of the Macromolecular Division of the Korean Chemical Society

Jung-Il Jin

Department of Chemistry, Korea University, Korea

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-2**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 16:00

Chair: Changjin Lee (KRICT)

Synthesis and Characterization of Photosensitive Polymers

Woo-Sik Kim

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

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-3**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 16:20

Chair: Changjin Lee (KRICT)

Fascinating Polymer and Life

Won Jei Cho

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

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-4**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 16:40

Chair: Changjin Lee (KRICT)

A Glimpse of Photoresist Materials Chemistry in Advancing Photolithography during the Last 30 Years

Kwang-Duk Ahn

Korea Institute of Science and Technology, Korea

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-5**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 17:00

Chair: Changjin Lee (KRICT)

A Half Centennial Story of Polymer Researches - From Nylon-4 to Polyimides

Kil-Yeong Choi

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

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **POLY1-6**

Symposium for Polymer Division 30th Anniversary

Room 325C+D, THU 17:20

Chair: Changjin Lee (KRICT)

Molecular and Structural Characterization of Polymers

Taihyun Chang

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

Symposium : **POLY2-1**

Recent Trends in Polymer-Based Therapeutics

Room 325C+D, FRI 14:30

Chair: Eunji Lee (GIST)

Peptidomimetic Polyethers: Model Study with Mussel and Frog

Byeong-Su Kim

Department of Chemistry, Yonsei University, Korea

Recent advances in synthetic polymer chemistry have allowed the generation of simple, protein-like structures with biological activity from synthetic designer polymers. To mimic the biological functions of the natural proteins, many synthetic approaches have incorporated vinyl monomers bearing the constitutional amino acid residues found in nature. However, since vinyl monomers have an all-carbon backbone, they are structurally rigid and have an intrinsic limitation in aqueous solubility. These factors often pose a challenge for creating systems that have the full potential to mimic natural polypeptides. Unlike many other existing approaches in the literatures, herein we present to employ functional polyethers bearing amino acid side chains. Toward this end, we developed a library of a new class of well-defined, functional epoxide monomers, which are polymerized into functional peptidomimetic polyethers. The integration of a flexible polyether backbone coupled with amino acid moieties will offer several advantages for materials and biomedical fields: (a) functional group availability resulting in improved hydrophilicity in biomimetics, and (b) capability of self-assembly to form hierarchical superstructures. Two specific examples toward mimicking the marine mussel foot proteins and the antimicrobial peptides secreted from frog will be presented with their future biomedical applications.

Symposium : **POLY2-2**

Recent Trends in Polymer-Based Therapeutics

Room 325C+D, FRI 15:00

Chair: Eunji Lee (GIST)

High-Accuracy Tumor Detection In Vivo by Fluorescence Imaging Using Neural Stem Cells Loaded with Reversibly Photoswitchable Nanoclusters

Yoonkyung Kim

Division of Biomedical Sciences, Korea Research Institute of Bioscience and Biotechnology, Korea

Fluorescence imaging is a convenient, safe, and relatively inexpensive method that is frequently used in biological studies. For biomedical applications, various types of nano-sized fluorescent compounds have been made to detect diseases such as cancer. Targeting of tumors by intravascularly administered nano-sized fluorophores is generally accomplished via multivalent interactions between their surface-bound ligands and the tumoral receptors (i.e., active targeting), or/and the enhanced permeability and retention (EPR) effect (i.e., passive targeting). Unfortunately, the clinical use of these nano-sized fluorophores is yet limited, mainly because of the penetration depth of light, autofluorescence, and poor tumor-targeting efficiencies. Here we demonstrate a highly reliable strategy to detect tumors in living systems using the reversibly photoswitchable fluorescent dendritic nanoclusters (ca. 20 nm in diameter), which were made by crosslinking biocompatible dendrimers with photochromic diarylethene derivatives. Specifically, the high accuracy of tumor detection was successfully achieved by 1) utilizing tumor tropic neural stem cells as vehicles to correctly deliver our dendritic nanoclusters to the tumor site, and 2) executing reversible photoswitching to distinguish the fluorescence of our compounds from the autofluorescence in the in vivo environment. We envision that our method to detect tumors can significantly improve the reproducibility of the fluorescence-based diagnostic imaging in cancer nanomedicine.

Symposium : **POLY2-3**

Recent Trends in Polymer-Based Therapeutics

Room 325C+D, FRI 15:30

Chair: Eunji Lee (GIST)

Design of biopolymer-based brain gel for highly effective soft neural interface

Yong Ho Kim

Department of Chemistry, SKKU Advanced Institute o, Sungkyunkwan University, Korea

Recording neural activity from live brain is of great interest in neuroscience for interpreting cognitive processing or disease states of neurological disorders. However, soft neural interface that allows a tight integration with neural tissues to increase recording sensitivity and prevent signal dissipation is yet to be achieved. In this talk, I introduce a biocompatible, conductive, and biostable neural interface with supramolecular β -peptide-based hydrogel that allows signal amplification via seamless neural/hydrogel contact. The peptide, which consists of non-biodegradable β -amino acids, formed multi-hierarchical structure with conductive nanomaterial to construct three-dimensional electrical network in the hydrogel. The intercortical and epidural neural signal recorded with the hydrogel were founded to be augmented, especially in high frequency range, due to increased contact area and tight coupling with neural tissues. Our results suggest that tissue-like soft neural interface will facilitate deep understanding on brain oscillation in broad brain states.

Symposium : **POLY2-4**

Recent Trends in Polymer-Based Therapeutics

Room 325C+D, FRI 15:55

Chair: Eunji Lee (GIST)

Polymerized Nucleic Acid Nanoparticles for Anticancer Drug Delivery

Young Hoon Roh

Department of Biotechnology, Yonsei University, Korea

Herein we introduce size-tunable and tumor-targetable nucleic acid nanocarriers that combine the cargo and carrier for anticancer drug delivery. These nucleic acids nanocarriers consist of cleavable polymeric nucleic acid strands by rolling circle replication, inherently providing protection for cancer therapeutics during delivery and transport to the cytoplasm and nucleus. In addition, packaging multiple polymeric nucleic acid molecules into microstructures at precisely defined types and ratios is possible as a powerful delivery strategy for effective RNA interference (RNAi). Furthermore, by employing layer-by-layer (LBL) assembly, these nucleic acid microstructures can further condense and re-assemble with tunable surface charge and size. These LbL platforms are equipped with multi-functional properties, resulting in an improved imaging, targeted intracellular uptake, and powerful therapeutic potency with negligible cytotoxicity compared to traditional synthetic vectors toward specific diseases and tumor targets. These formulations also significantly improve nucleic acid drug/carrier stability as well as plasma half-life during in vivo biodistribution ensuring meaningful delivery to targeted tissues. These nucleic acid nanotechnology-based approaches can lead to novel therapeutic routes for cancer therapy.

Symposium : **POMA-1**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 09:00

Chair: Hyosung Choi (Hanyang University)

High performance epoxy resins and chemical recycling of epoxy based composites

Munju Goh

Institute of Advanced Composite Materials, Korea Institute of Science and Technology, Korea

Epoxy resin (EP), the most common thermosetting resin, forms a three-dimensional cross-linked network structure. EP has been used in various industrial applications because of its good adhesion, chemical resistance, thermal resistance, and mechanical properties. Despite its good properties, there has been a persistent demand for more functional EP that can be used in potential applications such as in automotive, aerospace, construction, and electronic industries. In this presentation, I will describe recent progress for enhancing the crosslink density, glass transition temperature and mechanical properties of EP using nanocarbon materials as a curing agent and synthesizing highly thermal conductive epoxy resins. Finally, I introduce a new chemical recycling method that overcomes the disadvantages of thermosetting resins that cannot be recycled because they are insoluble and infusible after curing.

Symposium : **POMA-2**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 09:20

Chair: Hyosung Choi (Hanyang University)

Multi-Functional Nanomaterials and Nanotechnology for Next Generation Energy Applications

Dong Hwan Wang

College of ICT Engineering School of Integrative E, Chung-Ang University, Korea

Recently, stamping transfer technology using by thin films or soft mold has been considered by advanced technology to overcome limits of wet coating such as spin or dip coating, which are composed of deposition of large area and specific region, the material loss, and penetration of solvents. In this research, we investigated stamping transfer via polyurethane acrylate (PUA), of which the surface energy was modified by 2-hydroxyethyl methacrylate (HEMA) to increase the transfer reproducibility. As a results, hydrophilic PUA was used to form organic bulk hetero junction (BHJ) layer onto PEDOT:PSS/ITO substrates. The transferred device revealed a comparable efficiency, 95% relative to spin coating device. In order to find a decrease of fill factor of transferred device, we observed charge recombination and resistance through impedance spectroscopy. Furthermore, we applied stamping transfer to formation of interlayer in planer-type perovskite photovoltaic cells. We have successfully fabricated the device with transferred inter-layer, 6,6-phenyl-C71 butyric acid methyl ester (PC71BM), onto perovskite layer by dry stamping transfer condition. The device exhibited enhanced Jsc and efficiency, which were caused by improved coverage of inter-layer on perovskite layer, correlated with increased electron mobility and exciton dissociation.

Symposium : **POMA-3**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 09:40

Chair: Hyosung Choi (Hanyang University)

Tetraphenylimidazole and triphenylamine-based simple hole-transporting materials for efficient perovskite-solar cells

Sanghyuk Park

Department of Chemistry, Kongju National University, Korea

In organic hole-transporting material(HTM)-based p-i-n planar perovskite solar cells (PSCs), which have simple and low-temperature processibility feasible to low-cost flexible PSCs, the incident light has to pass through the HTM before reaching the perovskite layer. Therefore, photo-excited state of organic HTM could become important during the solar cell operation, but this feature has never been considered for the HTM design until now. In this work, we prove that designing organic HTMs to have the enhanced property at their photo-excited states could be a new methodology to improve their performances for the high efficiency p-i-n PSCs. Especially, we focus on their transition dipole moment variation at the photo-excitation and firstly develop a design principle of organic HTMs, which can intensify this feature by the excited-state intramolecular proton transfer (ESIPT) process, for the high performance p-i-n planar PSCs. Following the design rules, different from the conventional HTMs such as spiro-OMeTAD and PTAA, organic HTMs can be designed to have high dipole moment at the excited states, and this property can be preserved during the solar cell operation due to their extended lifetime by the ESIPT process, consequently improving the charge recombination and extraction property of PSC devices. Moreover, their UV-filtering ability is beneficial to enhance the photostability of PSCs. We believe that our suggestion could be a new strategy to design efficient HTMs for high performance PSCs.

Symposium : **POMA-4**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 10:00

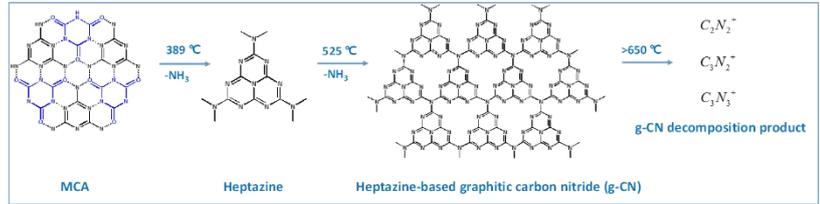
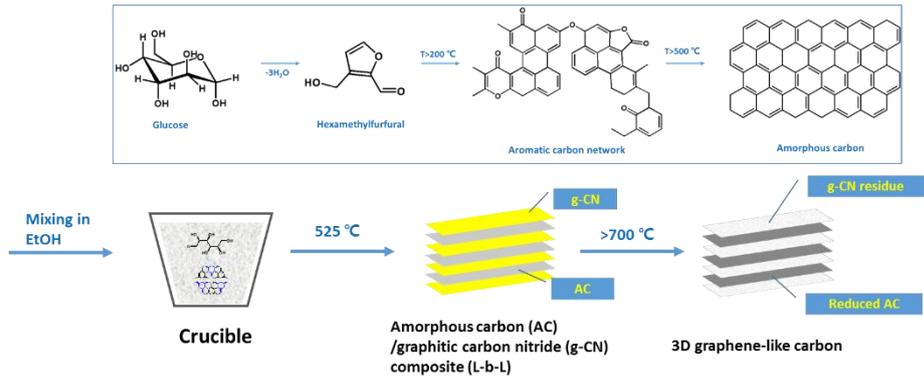
Chair: Daehwan Park (Kyungnam University)

High performance Na hybrid capacitors: from pre-organized triazine crystals to nitrogen-rich hard carbons

Young-Si Jun

School of Chemical Engineering, Chonnam National University, Korea

Next-generation flexible energy storage systems must simultaneously be cheap, flexible, and durable upon repeated flexing as well as offer high energy/power density. Although LIBs provide high energy density and offer a variety of cell form factors, their low power density and price issues, resulting from sluggish intercalation/de-intercalation kinetics and a mismatch between rapidly-growing demand and limited reserves, respectively, pose a significant challenge to expand into the future flexible electronics. Such considerations give rise to an emerging electrochemical energy storage system, i.e. flexible hybrid capacitors based on earth-abundant and low-cost sodium, which could deliver energy at much higher currents and lower costs than LIBs. In order to further improve capacity and rate capability of sodium hybrid capacitors, we develop a versatile synthesis strategy of high performance hard carbon electrode based on pre-organized reactive templates. Shape and size controllable organic crystal of melamine and cyanuric acid hydrogen bonded aggregates (MCA) as reactive templates performs triple duties of (1) structure directing agent, (2) nitrogen source, and (3) porogen. Ratio of MCA to glucose (matrix forming agent) simply controls interlayer spacing, lateral size, and stacking height of graphitic domain, ratio of graphitic to non-graphitic content, nitrogen content, and porosity. This unique structure enables a gravimetric capacity of 389 mAh/g at a high current density of 250 mA/g over 100 cycles, rendering it one of the best hard carbon anode for Na-ion. Hybrid capacitor consisted of the hard carbon anode and activated carbon fiber cathode feature a gravimetric energy density of 220 Wh/kg and a power density of 1000W/kg.



Symposium : **POMA-5**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 10:20

Chair: Daehwan Park (Kyungnam University)

Water-Resistant Conjugated Polymer Film by Photo-Crosslinking Agent for Solution-Processable Thin Film Solar Cells

Hyosung Choi

Department of Chemistry, Hanyang University, Korea

We report a water-resistant PEDOT:PSS HTL by incorporating a photo-crosslinking agent into a PEDOT:PSS film. A crosslinking system was successfully formed inside the PEDOT:PSS film by simple and fast photo-polymerization of PCDSA monomers. Combination of the crosslinking system and MeOH surface treatment simultaneously improved the device efficiency and stability of both perovskite and polymer solar cells. The crosslinking system inside PEDOT:PSS changed its intrinsic water-soluble characteristic into a water-resistant property, thus preventing water penetration into the PEDOT:PSS film. In addition, MeOH treatment improved the surface conductivity and reduced the surface roughness of the PEDOT:PSS film by removing surface residues of PDAs and insulating PSS parts.

Symposium : **POMA-6**

[Polymer Chemistry - Material Chemistry Divisions Joint Symposium] Organic/Inorganic/Polymer Hybrids

Materials: Present and Future

Room 325C+D, FRI 10:40

Chair: Daehwan Park (Kyungnam University)

Probing Interfacial Structure in Organosilica Nanochannels by Solid State NMR

Young Joo Lee

Institute of inorganic and applied chemistry, University of Hamburg, Germany

Periodic mesoporous organosilica (PMO) are inorganic-organic hybrid materials which combine the advantages of functional variation of organic chemistry and thermal and mechanical robustness of inorganic substance. These materials are characterized by large surface area and pore sizes ranging between 2 and 15 nm, enabling applications in versatile area such as catalysis, sensor, energy storage, adsorption, chromatography etc. To develop new materials with desired properties for various applications, fundamental understanding of the materials is necessary, in particular, the influence of pore wall chemistry on the interaction with guest molecules. Solid state NMR spectroscopy is an ideal tool to get structural and dynamic information of materials even when long-range order is lacking such as amorphous and glassy materials. In this presentation, we will present solid state NMR study on the host-guest interaction and interfacial structure of confined water and surfactant in mesopores of PMO. By changing organic bridge groups with different functionality, the effect of surface polarity on the interfacial structure, confinement effect and formation mechanism will be explored.

Symposium : **INORI-1**

Bioinorganic Chemistry (Metals in Biology)

Room 323, THU 15:40

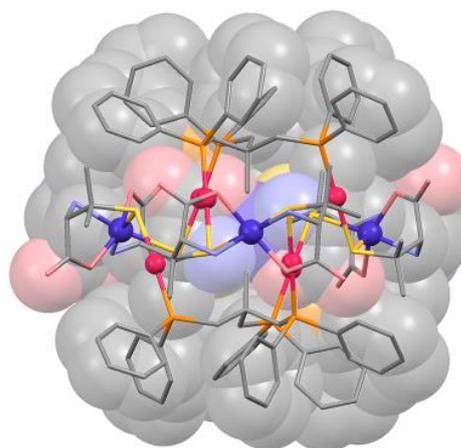
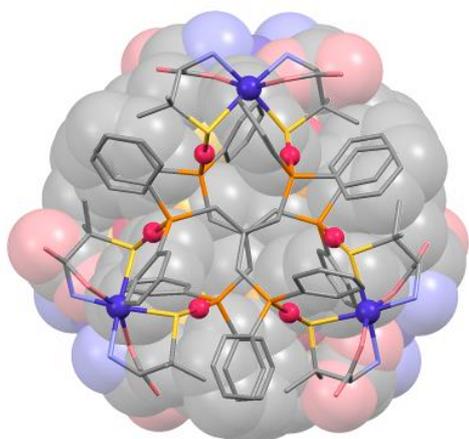
Chair: Mi Hee Lim (KAIST)

Coordination Behavior of Gold(I) Metalloligands with Thiol-containing Amino Acids

Takumi Konno

Department of Chemistry, Graduate School of Science, Japan

Heterometallic coordination compounds that contain more than one kind of metal ions and their supramolecular aggregates have attracted considerable attention in the fields of coordination chemistry and supramolecular chemistry. This class of compound is commonly synthesized by the one-step self-assembly of well-designed organic ligands in combination with a mixture of metal ions, which often results in the formation of undesired products. To overcome this issue, we have developed a metalloligand approach, in which a pre-designed metal complex with several donor sites is stepwise reacted with metal ions.¹ For example, we have shown that $[\text{Au}(\text{D-pen-S})_2]^{3-}$ ($\text{H}_{2\text{pen}}$ = penicillamine) acts as a multidentate metalloligand to produce a variety of heterometallic coordination compounds. Recently, this monogold(I) metalloligand system was extended to digold(I) and trigold(I) systems by introducing a digold(I)/trigold(I) linker with diphosphine/triphosphine ligands.² Here we present the coordination functionality of these metalloligands, which lead to the construction of unique metallosupramolecular architectures. References 1. a) Oji, K.; Igashira-Kamiyama, A.; Yoshinari, N.; Konno, T. *Angew. Chem. Int. Ed.* **2014**, *53*, 1992-1996; b) Yoshinari, N.; Kakuya, A.; Lee, R.; Konno, T. *Bull. Chem. Soc. Jpn.* **2015**, *88*, 59-68; c) Surinwong, S.; Yoshinari, N.; Kojima, T.; Konno, T. *Chem. Commun.* **2016**, *52*, 12893-12896; d) Kuwamura, N.; Kurioka, Y.; Konno, T. *Chem. Commun.* **2017**, *53*, 846-849; e) Kouno, M.; Yoshinari, N.; Kuwamura, N.; Yamagami, K.; Sekiyama, A.; Okumura, A.; Konno, T. *Angew. Chem. Int. Ed.* **2017**, *56*, 13762-13766. 2. a) Yamada, M.; Yoshinari, N.; Kuwamura, N.; Saito, T.; Harano, K.; Nakamura, Sekiyama, A.; Suenobu, T.; Yamada, Y.; Konno, T.; *Chem. Sci.*, **2017**, *8*, 384-386; b) Itai, T.; Kojima, T.; Kuwamura, N.; Konno, T. *Chem. Eur. J.* **2017**, *23*, 16438-16441; c) Yamashita, S.; Nakazawa, Y.; Yamanaka, S.; Okumura, M.; Kojima, T. Konno, T., *Sci. Rep.* **2018**, *8*, 2606.



Symposium : **INORI-2**

Bioinorganic Chemistry (Metals in Biology)

Room 323, THU 16:10

Chair: Mi Hee Lim (KAIST)

Selective Conversion of CO₂ to CO at a Single Nickel Center

Yunho Lee

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

Carbon dioxide conversions mediated by transition metal complexes continue to attract much attention due to its potential utilization as a C1 source for the future industry. One of the main challenges in transition metal-based CO₂ catalysis is to accomplish the high selectivity in producing a desired product. This may rely on the interaction of CO₂ with a metal center. Given the presence of nickel in natural systems that allow for extremely efficient catalysis, studies that focus on selective CO₂ conversion to CO with synthetic nickel species are currently of considerable interest in our group. The chemistry is inspired by an efficient enzymatic CO₂ catalysis occurring at the active site of the carbon monoxide dehydrogenase (CODH). Since the binding and reactivity toward CO₂ is controlled in part by the geometry of a L₃Ni scaffold, we have explored the chemistry of low-valent nickel supported by pincer systems (E = P or N), in which a pseudo-tetrahedral or square planar geometry is accommodated. The central donor atom is P for a PPMeP ligand (PPMeP = PMe[2-PiPr₂-C₆H₄]₂) and N for PNP (PNP⁻ = N[2-PiPr₂-4-Me-C₆H₃]₂⁻) and acriPNP ligands (acriPNP⁻ = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide). Two isolated nickel-CO₂ adducts, (PPMeP)Ni(η²-CO₂-κC) and {Na(12-C-4)₂}{(PNP)NiCO₂}, demonstrate that the geometry of a nickel ion is crucial in the binding of CO₂ and its level of activation. In the case of a square planar nickel center, a series of bimetallic metallacarboxylate Ni-μ-CO₂-κC,O-M species (M = H, Na, Ni or Fe) were synthesized and studied. Protonation cleaves the C-O bond in the nickel(II)-carboxylate species resulting in the formation of a nickel(II) monocarbonyl complex. By sequential reduction, the corresponding mono- and zero-valent Ni-CO species were generated. In particular, a (PNP)Ni(0)-CO species shows immediate reactivity toward CO₂ but displays the formation of multiple products. With a structurally rigidified acriPNP ligand, the Ni(0)-CO species reveals the selective addition of CO₂ to give a nickel(II)-carboxylate species with the expulsion of CO. The closed synthetic cycle for CO₂ reduction to CO was finally established with a (acriPNP)Ni system.

Symposium : **INOR1-3**

Bioinorganic Chemistry (Metals in Biology)

Room 323, THU 16:35

Chair: Mi Hee Lim (KAIST)

Regulation of hydroxylase activity through auxiliary components in metallo-enzymes

Seung Jae Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Chonbuk National University, Korea

Hydroxylation through soluble methane monooxygenase (sMMO) has been studied extensively to understand the biological conversion from methane to methanol in ambient conditions, although more detailed mechanisms of this biocatalyst are yet undiscovered. In this study, sMMO components, including the hydroxylase (MMOH), regulatory (MMOB), and reductase (MMOR), were expressed and purified from a type II methanotroph, *Methylosinus sporium* strain 5 (*M. sporium* 5), to characterize its hydroxylation mechanism. Brown-black pigments were detected in *M. sporium* 5 during cell growth, with the optical density value of 8.0 at 600 nm (OD₆₀₀), and this change was dependent on the ratio of cell:iron. The cell extract showed that MMOH, MMOB, and MMOR were expressed by *M. sporium* 5, and these enzymes were extracted with high purity. The enzyme activity confirmed that 2.0 mol equivalents of MMOB is necessary to achieve catalytic activities, and sMMO from *M. sporium* 5 oxidized a broad range of substrates, including alkanes, alkenes, halogens, and aromatics. Optimal activities were observed at pH 7.5 in most substrates, possibly because of the electron transfer environment in MMOR, and this was explained by the optical spectra from FAD-containing domains. The substitution of MMOB or MMOR from another type II methanotroph, *Methylocystis species M* (*M. species M*), retained specific enzyme activities, demonstrating the successful crossreactivity of *M. sporium* 5. These characterizations will provide fundamental information for further enzymatic studies to acquire biophysical information to elucidate sMMO mechanisms.

Symposium : **INOR1-4**

Bioinorganic Chemistry (Metals in Biology)

Room 323, THU 17:00

Chair: Mi Hee Lim (KAIST)

Application of Advanced EPR Spectroscopy for Bio-inorganic Chemistry

Sun Hee Kim

Western Seoul Center, Korea Basic Science Institute, Korea

EPR spectroscopy has been proven to play a significant role to characterize paramagnetic species. For example, metal ions in metalloenzymes are reactive centers for various fascinating catalytic reactions that nature has shown us. Thus, to investigate these metal ions and radical cofactors, which is paramagnetic, EPR spectroscopy has been fruitfully exploited. Our group utilizes advanced EPR spectroscopy, i.e. multi-frequency, multi-technique pulse EPR, (for the first time in Korea) to elucidate molecular mechanisms of bio-catalysts by placing an emphasis on revealing structures of intermediates of interesting biomolecules. In addition, advanced EPR spectroscopy provides accurate spin Hamiltonian values which can be used for explanation of the electronic structures of short-lived intermediates species via in-depth analysis, hence may deepen our knowledge for understanding working mechanisms of the interesting catalytic reactions. In this talk, I will present case studies of application of advanced EPR spectroscopy, the recent results from our group. These include structural studies of ternary complex of metal, amyloid peptide and a chemical regulator and metal-oxo species as an intermediate of catalytic reactions.

Symposium : **INOR2-1**

Recent Research Activities in Solid-State Materials

Room 323, FRI 09:00

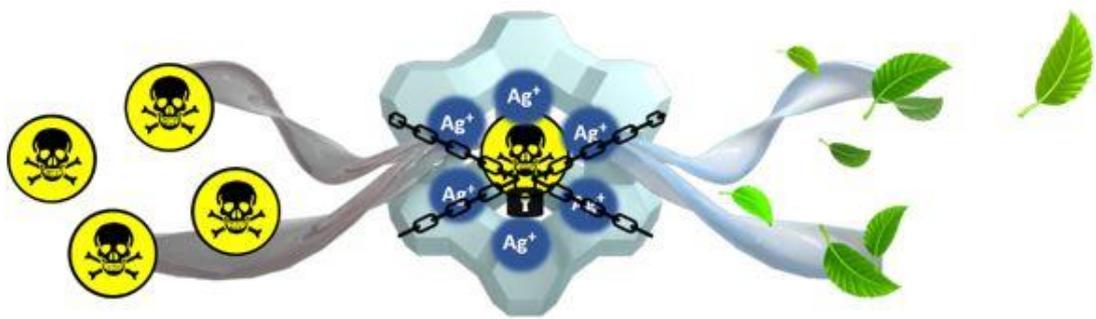
Chair: Minyoung Yoon (Gachon University)

Zeolite based decontaminants against chemical warfare agents

Hyun Sung Kim

Department of Chemistry, Pukyong National University, Korea

The recent turmoil and volatile situation in many countries and the increased risk of terrorist activities have raised alarm bells for the field of defense against toxic chemical/materials. These situations pose threats to society as terrorists can take advantage of such situations to strike and cause public mayhem. We will introduce briefs about different decontamination processes and approaches for chemical decontamination and also discuss about various decontamination products available globally. Especially, sulfur mustard gas, also called HD, is one of the main chemical warfare agents and has claimed thousands of lives and left many more contaminated. The development of functional materials to promptly capture and detoxify sulfur mustard within a few minutes is extremely important to save the lives of the affected people. This has motivated us to explore excellent detoxification systems that can be deployed in the field to rapidly capture and hydrolyze mustard gas in a short time. To that end, we present a silver-ion-exchanged zeolite Y $[(Ag^+)_n@Y, n = 5, 13, 21, 32, 43 \text{ and } 55]$ that can rapidly capture mustard gas and its simulant (2-chloroethyl ethyl sulfide, CEES) in ambient conditions to enable the prompt hydrolysis of the CEES captured in its nanopores.



Ag⁺ exchanged zeolite Y

Symposium : **INOR2-2**

Recent Research Activities in Solid-State Materials

Room 323, FRI 09:20

Chair: Minyoung Yoon (Gachon University)

Carbon-based composite materials for electrochemical applications

Won Cheol Yoo

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Carbonaceous materials possess fascinating properties such as high surface area, controllable pore size distribution (PSD), high electric conductivity, light weight, possible heteroatom-doping, surface functionalization, and chemical & physical stability; therefore they have widely been utilized as adsorbents, electrode materials, as well as templates/supports for composite materials for synergic effects. In this presentation, design and synthesis of porosity and polarity controlled carbon-based composite materials employed as electrocatalysts for oxygen reduction reaction (ORR) and electrodes for supercapacitors will be discussed.

Symposium : **INOR2-3**

Recent Research Activities in Solid-State Materials

Room 323, FRI 09:50

Chair: Tae-Soo You (Chungbuk National University)

Solution Processing of Scalable Metal-Chalcogenide Semiconductors for Large Area Electronics

Myung-Gil Kim

Department of Chemistry, Chung-Ang University, Korea

In modern daily life, the large area display have been the major information delivery media for internet and broadcasting. Furthermore, as represented by the recent development of high performance thin-film solar cell, ubiquitous sensor array for personal health care, and internet of things, the emerging large area electronics applications requires development of high performance semiconducting materials for emerging applications. Metal chalcogenide have been known as promising materials for electronics and solar cell applications. Although there have been limited success of solution processing of metal chalcogenides, The general strategy for obtaining high-quality, large-area metal chalcogenide semiconductor films from soluble precursors is still under development. In this talk, I will present the recent development of high performance metal chalcogenide semiconductors with soluble molecular precursor and nanomaterials. The optimized TFT device could exhibit a maximum field-effect mobility greater than $300 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ with an on/off current ratio of $> 10^7$ and a good operational stability (threshold voltage shift $< 0.5 \text{ V}$ at positive gate-bias stress of 10 ks). In addition, metal-chalcogenide-based seven-stage ring oscillators operating at an operating speed of $\sim 2.6 \text{ MHz}$ (propagation delay of $< 27 \text{ ns/stage}$) was demonstrated.

Symposium : **INOR2-4**

Recent Research Activities in Solid-State Materials

Room 323, FRI 10:10

Chair: Tae-Soo You (Chungbuk National University)

Solid state materials with noncentrosymmetric structures revealing very large second-harmonic generation response

Kang Min Ok

Department of Chemistry, Chung-Ang University, Korea

A series of new solid state materials crystallizing in macroscopic noncentrosymmetric (NCS) crystal structures are introduced. Various starting reagents containing important NCS chromophores such as two families of second-order Jahn-Teller (SOJT) distortive cations, π -delocalized anionic groups, π -localized distorted groups, and highly polarizable cations have been utilized in the initial synthesis reactions in order to maximize the second-harmonic generation (SHG) response. Detailed crystal structures of the newly discovered solid state materials have been determined via single crystal X-ray diffraction. Structure-SHG property relationships as well as other physical properties of novel materials with NCS structures such as variable band gaps and thermal stability are also elucidated. The structural origin of exceptionally strong SHG response and the interesting synergistic effect found from the constituent NCS chromophores are discussed.

Symposium : **INOR2-5**

Recent Research Activities in Solid-State Materials

Room 323, FRI 10:30

Chair: Tae-Soo You (Chungbuk National University)

Data-Driven Discovery of New Porous Materials

Wonyoung Choe

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

From state-of-art meta materials and catalysts for petrochemical industries, porous materials play important roles in science and industries. A rising subclass of porous materials includes zeolitic imidazolate frameworks (ZIFs). Despite strong structural similarities between these ZIFs and zeolites, only limited numbers of ZIFs are synthetically accessible. In this presentation, we show how hypothetical zeolite databases can be helpful to identify possible ZIF structures, utilizing simple chemical descriptors, and discuss the impact of such data-driven approach for accessing new porous materials.

Symposium : **INOR3-1**

Recent Trends in Catalysis Based on Nano-Porous Inorganic Materials

Room 323, FRI 14:30

Chair: Chang Yeon Lee (Incheon National University)

Design Strategy toward Recyclable and Highly Efficient Heterogeneous Catalysts for the Hydrogenation of CO₂ to Formate

Sungho Yoon, Seok-Chan Kim^{1,*}, Gyoosoon Park^{1,*}

Department of Applied Chemistry, Kookmin University, Korea

¹*Department of Chemistry, Kookmin University, Korea*

One bottleneck in the realization of CO₂ conversion into value-added compounds is the lack of catalysts with both excellent activity and recyclability. Herein, a catalyst is designed for the hydrogenation of CO₂ to formate to boost up these features by considering the leaching pathway of previously reported heterogenized catalyst; the design strategy incorporates oxyanionic ligand(s) in the coordination sphere to provide a pathway for both preventing the deleterious interactions and assisting the heterolysis of H₂. The tailored heterogenized catalyst, [bpy-CTF-Ru(acac)₂]Cl, demonstrated excellent recyclability over consecutive runs with a highest turnover frequency of 22 700 h⁻¹, and produced a highest formate concentration of 1.8M in 3h. This work is significant in elucidating new principles for the development of industrially viable hydrogenation catalysts.

Symposium : **INOR3-2**

Recent Trends in Catalysis Based on Nano-Porous Inorganic Materials

Room 323, FRI 15:00

Chair: Chang Yeon Lee (Incheon National University)

Transfer Hydrogenation of Biobased aldehyde to alcohol over MOF

Young Kyu Hwang

Korea Research Institute of Chemical Technology, Korea

Enormous efforts are being made to develop suitable catalytic processes for the production of various platforms and value-added chemicals from carbohydrate, or directly from lignocellulosic biomass. Among these chemicals, γ -Valerolactone (GVL) is recognized as a versatile building block that could be utilized as an additive in liquid fuel for transportation, as precursor for the production of polymeric monomers, and for creation of various value-added chemicals including organic solvents and bio-oxygenates. GVL itself has proved an excellent green solvent for biomass processing due to its extraordinary physicochemical properties, which include low melting and high boiling points; remarkably low vapor pressure, even at elevated temperature and its ready miscibility with water without forming an azeotropic mixture. In this work, a series of zirconium MOFs were selected to study the catalytic transfer hydrogenation (CTH) of EL to GVL using isopropanol as H-donor. Isopropanol has already been proven as the preeminent H-donor alcohol due to its low reduction potential. It is believed that EL should be the preferred choice over LA for GVL production for two reasons. In this talk, we will also show another example for CTH based on heterocyclic aldehyde feedstock.

Symposium : **INOR3-3**

Recent Trends in Catalysis Based on Nano-Porous Inorganic Materials

Room 323, FRI 15:30

Chair: Chang Yeon Lee (Incheon National University)

Localized basification of the mesopore walls as a route to high dispersion of supported-metal catalyst

Changbum Jo, Jangkeun Cho¹, Ryong Ryoo^{2,*}

Center for Nanomaterials and Chemical Reactions, Inha University, Korea

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

²*Center for Nanomaterials and Chemical Reactions, Institute for Basic Science, Korea*

Development of a simple and scalable protocol for the high dispersion of supported metal nanoparticles is an important aspect in catalysis. Most water-soluble inorganic salts become insoluble when adding base into the aqueous solution; therefore, we have attempted to induce localized precipitation of inorganic species onto the mesopore walls via surface basification with $-(\text{Me}_4\text{N}^+)(\text{OH}^-)$ or $-\text{NH}_2$ groups. Herein, we demonstrate that a high content (~30 wt.%) of Ni, Cu, SnO nanoparticles can be highly dispersed on the mesopore walls functionalized with $-(\text{Me}_4\text{N}^+)(\text{OH}^-)$ or $-\text{NH}_2$ groups. As a result of high dispersion, the metal nanoparticles supported on mesoporous zeolites exhibited a high catalytic activity in CO_2 methanation reaction. This strategy can be generalized to various supports, such as MFI zeolite nanosponges, a MCM-48 mesoporous silica, and a mesoporous alumina. We believed that the basic-surface induced precipitation would be an effective way to increase the metal-surface sites, and consequently, advanced catalytic function in a number of applications.

Symposium : **INOR3-4**

Recent Trends in Catalysis Based on Nano-Porous Inorganic Materials

Room 323, FRI 15:55

Chair: Chang Yeon Lee (Incheon National University)

Porphyritic MOFs Driven Photocatalytic CO₂ Reduction: Efficient Energy Migration from MOFs to Reduction Center

Ho-Jin Son

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

A porphyritic metal-organic framework (PMOF) known as PCN-222 was surface-modified by the molecular Re(I) catalyst through anchoring to the outer layer with carboxylate to form a new type of MOF hybrid photocatalyst. The porphyritic MOF-based hybrid (PMOF|Re) prepared with an archetypical CO₂ reduction catalyst, (L)ReI(CO)₃Cl (Re(I); L = 4,4'-dicarboxylic-2,2'-bipyridine), in the presence of 3 vol% water produced CO with no leveling-off tendency for 32 h to give a turnover number of $\geq 533 \pm 57$ ($5,552 \pm 593 \mu\text{mol h}^{-1}$ (g MOF)⁻¹), which appears to be the highest reported for visible-light driven CO₂ reduction systems based on combination of MOF and Re(I) molecular complex. The resultant high TON on the catalytic activity should mainly arise from efficient electron transfer from photoexcited porphyrin linkers (ZnPs*) to the periphery Re(I) catalytic sites, which is in line with the observed amplified quenching behavior (~ ps) of photo-excited electrons toward Re(I) catalytic centers in PMOF|Re(I) hybrid (>7 $\mu\text{mol Re(I)/g PMOF}$). Such fast quenching might be expected to arise from energy (exciton) migration between porphyrin-like pigments (chlorophylls) and funneling into reduction site occurring in highly ordered porphyrin-based MOF|Re(I) hybrid, which is reminiscent of natural photosystem I. A protective coating of TiO₂ grown with post-treatment atomic layer deposition of TiO₂ (TiO₂-AIM) further improved the catalytic durability of this hybrid as a result of ALD-engendered structural strengthening of MOF, with its role as an electron mediator transferring the photo-excited electrons of PMOF toward the Re(I) reaction center.

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

Recent Trends in Energy Harvesting/Storage Systems

Room 324A, THU 15:40

Chair: Dongwook Kim (Kyonggi University)

Photosynthesis and Photoprotection in Plant and Artificial Cells

Tae Kyu Ahn

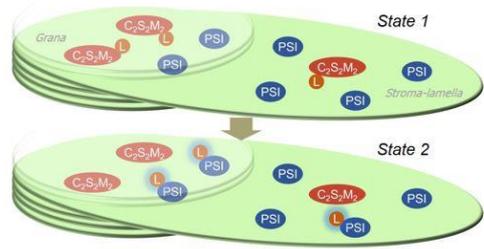
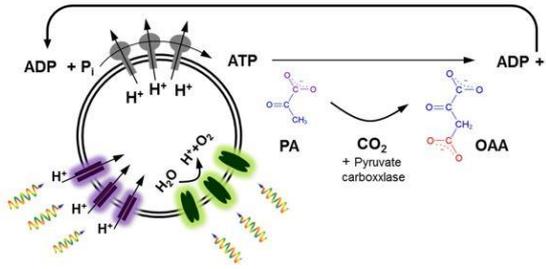
Department of Energy Science, Sungkyunkwan University, Korea

Complex metabolic reactions in cells are distributed in organelle modular compartments. Reactions in organelles have been reproduced in vitro by reconstituting functional protein machinery into membrane systems. We tested harvest organelle design, if switchable, to provide both a sustainable energy source and means to induce bladder response.[1] ATP (ATP) sinter agent and two light converters (plant-derived photochemical system II and proteorhodopsin derived from bacteria) enable ATP synthesis. It depends on two optical conversion devices, and it enables optical control to dynamically control ATP synthesis. Red light and green light interfere with ATP synthesis. We encapsulated giant vesicle light synthesizing organelle to form one cell line and showed two ATP dependent responses, optical control of carbon fixation and actin polymerization, changing the morphology of the vesicle. We hope to develop a full biomimetic vesicular system with a regulatory network showing switchable photosynthetic organelle homeostasis.

We applied fluorescence spectromicroscopy to Arabidopsis mesophyll protoplasts in order to observe in vivo changes in fluorescence spectra of granal and stromal thylakoid regions during the state transition, a photoprotection method. [2] State transition in chloroplasts of plants, is an important regulatory mechanism to maintain the excitation balance between PSI and PSII in the thylakoid membrane. Light-harvesting complex II (LHCII) plays a key role as the regulated energy distributor between PSI and PSII. The microscopic fluorescence spectra obtained from a few sections with different depths were decomposed into PSI and PSII spectra and self-absorption effects were removed. We determined amplitude changes of PSI and PSII in fluorescence spectra solely due to state transition. Subdomain analysis of granal and stromal thylakoid regions clarified variant behaviors in the different regions.

[1] Lee et al. Nature Biotechnology 2018, 36, 530–535.

[2] Kim et al. Plant Cell & Physiology 2015, 56, 759-768



Symposium : **PHYS1-2**

Recent Trends in Energy Harvesting/Storage Systems

Room 324A, THU 16:10

Chair: Dongwook Kim (Kyonggi University)

Nanoscale spatiodynamics of lithium-ion battery primary particles

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

Electrochemistry plays a significant role in energy storage and conversion technologies, such as lithium-ion batteries, fuel cells, and microbial fuel cells. Because of porous and heterogeneous nature of the electrodes in these applications, the conventional current-voltage measurement shows certain limit in untangling complexity of electrochemical reactions (charge transfer, mass transport, chemical reactions and so on). Here in my talk, I will introduce the in-situ electrochemical platform combined with synchrotron-based X-ray spectromicroscopy which visualizes nanoscale charge transfer and electrochemical reactions of individual battery particles.[1,2] Within individual particles, spatial variations in the electrochemical reaction rate control lithium ion insertion pathway. I will also discuss how this technique is expansively applied to other electrochemical systems in my group. [1] J. Lim et al “Origin and Hysteresis of Li Compositional Spatio-Dynamics within Battery Primary Particles”, Science, 2016, 353, 566-571[2] Y. Li et al “Fluid-enhanced Surface Diffusion Controls Intraparticle Phase Transformations” Nature Materials, 2018 in press

Symposium : **PHYS1-3**

Recent Trends in Energy Harvesting/Storage Systems

Room 324A, THU 16:35

Chair: Dongwook Kim (Kyonggi University)

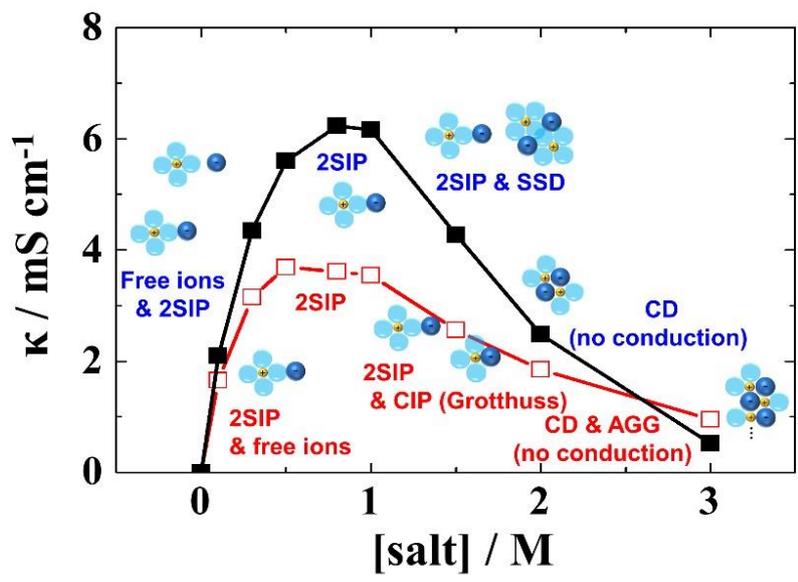
Ionic Conduction and Solution Structure of Li-ion Battery Electrolytes

Hochun Lee

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

Electrochemistry consists of two core fields: electrostatics and ionics. The electrostatics mainly deals with the charge transport at the electrified interface, while the ionics concerns on the ion transport and speciation in the ionic media. For the last century, the electrochemistry society has focused mainly on the electrostatics, whereas the ionics has seen no noticeable progress. This indifference to the ionics is partly due to the misunderstanding that the ionics is an old-fashioned field, and also due to the absence of the appropriate tools and theories. However, over the past decade, we have come to realize the importance of the ion conduction and solution structure in the concentrated electrolytes in developing energy storage/conversion devices (e.g., batteries, fuel cell, capacitors). At the same time, we are now lucky enough to enjoy remarkable advances in the analytical instruments and computing power, which now enable us to tackle the super-complex topic.

This talk will introduce some recent findings on the solution structure and ionic conduction behaviors in the Li-ion battery electrolytes including PC solutions of LiPF_6 and LiBF_4 and EC/linear carbonate solutions of LiPF_6 in an association with the ion-ion and ion-solvent interactions as investigated using Raman and pulse-field-gradient NMR measurements and a rather unfamiliar dielectric relaxation spectroscopy.



Symposium : **PHYS1-4**

Recent Trends in Energy Harvesting/Storage Systems

Room 324A, THU 17:10

Chair: Dongwook Kim (Kyonggi University)

Small Molecules Based Chemical Hydrogen Storage

Chang Won Yoon

Fuel Cell Research Center, Korea Institute of Science and Technology (KIST), Korea

To address the increasing global energy and environmental issues, safe and sustainable energy carriers alternative to carbon based fuels for the current power generation are being continuously investigated. One of the key issues for realizing the “hydrogen economy” is to develop reliable hydrogen storage/release systems that store/release large quantities of hydrogen in a safe and economically viable manner. Small molecules such as carbon dioxide (CO₂), nitrogen (N₂), and aromatic hydrocarbons are potential hydrogen storage media that can store hydrogen as liquid forms with high volumetric H₂ storage capacities, much higher than compressed hydrogen gas. In addition, the hydrogen atoms bonded to these small molecules can be released as H₂ gas in the presence of a proper catalyst. Despite these intriguing hydrogen release properties, highly active and selective heterogeneous catalysts for reversible hydrogen storage and release utilizing small molecules still remain challenges. Here, small molecules based hydrogen (energy) storage materials and related heterogeneous catalysts will be presented for different energy applications.

Symposium : **PHYS1-5**

Recent Trends in Energy Harvesting/Storage Systems

Room 324A, THU 17:35

Chair: Dongwook Kim (Kyonggi University)

Mesostructured Porous Carbons for Energy and Environmental Applications

Seung Jae Yang

Department of Chemical Engineering, Inha University, Korea

Porous carbons have a critical role in addressing the demands on energy- and environment-related issues due to their superior physic-chemical properties, wide availability, stability, and mass productivity. Considerable efforts have been made in porous carbon technology during the last decade to develop multi-functional nanostructured carbon materials, both through continuous ameliorant of pre-existing synthetic methods and through introduction of new technologies. In this presentation, however, I will introduce our new synthetic approaches for producing novel mesostructured carbons based on meso-crystals and metal-organic coordination. Mesostructured crystal based synthesis have provided advantageous hierarchical pore architecture with miscellaneous functionality in energy storage and pollutant removal systems. We will show an exemplified porous carbon synthesis based on carbon nitride mesostructure and energy storage application thereof. In addition, we will introduce a facile synthesis of highly-ordered mesostructured carbons based on metal-organic coordination. We presumed that these proposed synthetic approaches will provide a straightforward strategy to design the novel functioned porous carbons for making the promising candidates applicable to energy and environmental issues.

Symposium : **PHYS2-1**

Data-Enabled Computational Chemistry

Room 324A, FRI 09:00

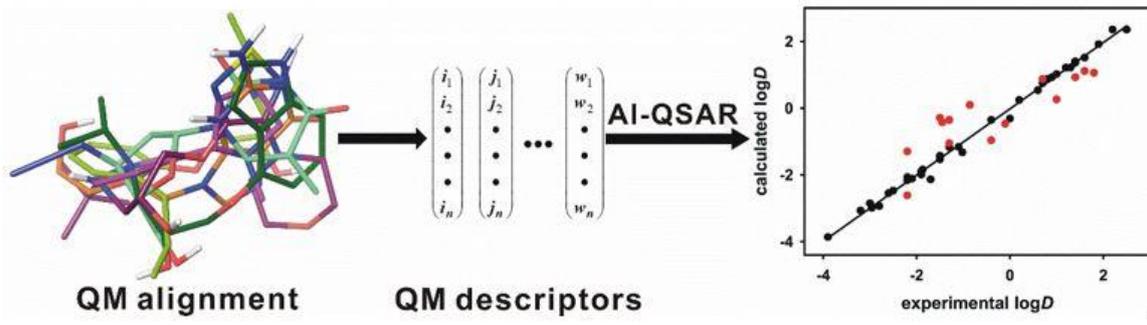
Chair: Yousung Jung (KAIST)

Development and Application of a Comprehensive Artificial Intelligence Program for Predicting Biochemical and Pharmacological Properties of Organic Molecules

Hwangseo Park

Department of Bioscience and Biotechnology, Sejong University, Korea

We establish a comprehensive quantitative structure-activity relationship (QSAR) model termed AlphaQ through the artificial intelligence algorithm to associate the fully quantum mechanical molecular descriptors with various biochemical and pharmacological properties. Preliminarily, a novel method for molecular structural alignments was developed in such a way to maximize the quantum mechanical cross correlations among the molecules. Besides the improvement of structural alignments, three-dimensional (3D) distribution of the molecular electrostatic potential was introduced as the unique numerical descriptor for individual molecules. These dual modifications lead to a substantial accuracy enhancement in multifarious 3D-QSAR prediction models of AlphaQ. Most remarkably, AlphaQ proves applicable to structurally diverse molecules to the extent that it outperforms the conventional QSAR methods in estimating the inhibitory activity against thrombin, the water-cyclohexane distribution coefficient, the permeability across the membrane of Caco-2 cell, and the metabolic stability in human liver microsomes. Due to the simplicity in model building and the high predictive capability for varying biochemical and pharmacological properties, AlphaQ is anticipated to serve as a valuable screening tool at both early and late stage of drug discovery.



Symposium : **PHYS2-2**

Data-Enabled Computational Chemistry

Room 324A, FRI 09:25

Chair: Yousung Jung (KAIST)

Classical neural network potential learning DFT results: a new frontier in physical chemistry

Wonseok Jeong, Seungwu Han*

Materials Science and Engineering, Seoul National University, Korea

By revealing atomic trajectories, classical molecular dynamics (MD) simulations have advanced fundamental understanding on various physical and chemical processes at the atomistic level. In classical MD, the chemical bonds are approximated by interatomic potentials that are parameterized by fitting key properties to reference data. The functional form of interatomic potentials reflects the underlying bonding nature. In many materials, however, the bonding nature is rather mixed, which makes it difficult to choose a proper function type. Recently, the machine-learning (ML) potential is gaining traction as a data-driven approach to generating interatomic potentials. In contrast to traditional interatomic potentials with preset analytic functions, the ML potentials assume flexible mathematical structures such as neural network and their parameters are optimized through machine learning on extensive reference data. While NNP is getting popular, the weakness and strength of NNP are not fully understood at this moment, mainly because of its 'black-box' nature. Here we show that NNP suffers from inhomogeneous feature-space sampling in the training set. As a result, underrepresented atomic configurations cause large errors even though they are included in the training set. Using the Gaussian density function (GDF) that quantifies the sparsity of training points, we propose a weighting scheme that can rectify the sampling bias. Various examples confirm that the GDF weighting significantly improves reliability and transferability of NNP compared to the conventional method, which is attributed to accurate mapping of atomic energies. By addressing a detrimental problem that is inherent in every ML potential, the present work will extend the application range of the ML potential.

Symposium : **PHYS2-3**

Data-Enabled Computational Chemistry

Room 324A, FRI 09:50

Chair: Yousung Jung (KAIST)

Deep learning for smart drug design

Woo youn Kim

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

The ultimate goal of materials and drug discovery is to create molecules with desired properties. This is obviously a difficult task because the molecular space is very large and discrete with a wide variety of molecules. For example, there are only 108 molecules synthesized, but 1060 molecules are estimated to be existing. Computer-aided molecular design is attracting attention as a promising solution for efficient materials and drug discovery. A fast calculation method allows us to find molecules with target properties through high-throughput virtual screening over known databases. As an alternative strategy, we propose to use a molecular generative model based on machine learning for de novo molecular design. It is specialized in controlling multiple molecular properties simultaneously, embedding them in namely the latent space. As a proof of concept, we will show that it can be used to generate a number of molecules as drugs with specific properties. We also apply it to design new molecules with promising binding energy for a specific target protein and use them as potential drug candidates that are not in the database.

Symposium : **PHYS2-4**

Data-Enabled Computational Chemistry

Room 324A, FRI 10:15

Chair: Yousung Jung (KAIST)

Design of Novel Catalysts: From First-Principles to Machine-Learning

Sang Soo Han

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

Electronic structures of materials such as electron densities of states (DOSs) are one of the most critical keys to determine material properties. Thus, prediction of the electronic structure using a first-principles density-functional theory (DFT) calculation has been regarded as a very useful tool for design of novel catalysts. Recently, a combination of the DFT calculation and the automation technique provides a high-throughput screening for a catalysis design. With this method, we have recently developed novel metallic catalysts for direct synthesis of hydrogen peroxide (H_2O_2), which shows a superior catalytic properties over the state of the art material, palladium (Pd). Moreover, the high-throughput screening technique is also efficient to build the DOS database, with which we can apply a machine-learning technique for design of novel catalysts. In this talk, we will also discuss the relevant recent advances.

On the other hand, although the DFT calculation provides an accurate DOS for a material, the calculation is very time-consuming. Herein, we will discuss a cost-effective method to predict the DOS of multi-component alloy systems based on a machine-learning algorithm called a principal component analysis, with which the shape of DOS can be even predictable. Within this framework, we input only a crystal structure and a composition. In comparison with the DFT calculation (GGA level), our machine learning method can provide the DOS results (both of value and shape) with an accuracy of >95% and a 1,000 times faster speed than the DFT calculation. To our best knowledge, this work is the first machine learning approach to predict the complete DOS information (value and shape) of multi-component alloys. In addition, we will introduce a neural network model for predicting binding energies of adsorbates on catalyst surfaces from the DOS. And, we have been recently developed a crystal graph convolutional neural network model for description of surface structures, which provides a novel way to predict such binding energies with no first-principles calculation information.

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

[KCS-GDCh Joint Symposium] Recent International Trends in Spectroscopic and Computational Chemistry

Room 324A, FRI 14:30

Chair: Kiyoung Park (KAIST)

Surface Science of 2-Dimensional Crystals Probed by Optical Spectroscopy

Sunmin Ryu

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

Two-dimensional crystals (2DX) represented by graphene hold substantial potentials both in fundamental research and industrial applications owing to their novel electronic and optical properties originating from dimensional confinement. In addition, their intrinsic properties are readily manipulated by chemical entities in direct contact because of their high fraction of surface atoms. To uncover and control emerging properties, my group has explored surface and interfacial science of low dimensional materials using various spectroscopic methods. Raman and photoluminescence spectroscopy, in particular, have proven to be versatile analytical probes because of their varying spectral features for different thickness, stacking, defect density, charge density, mechanical strain, temperature, etc. In this talk, I will share our past endeavor to understand important surface scientific problems in 2-dimension such as structural deformation caused by substrates and thermal perturbation, interfacial charge transfer, and molecular diffusion through 2DX-substrate interface.

Symposium : **PHYS3-2**

[KCS-GDCh Joint Symposium] Recent International Trends in Spectroscopic and Computational Chemistry

Room 324A, FRI 15:00

Chair: Kiyoung Park (KAIST)

Photoinduced mobile-carrier dynamics in semiconductors

JaeHong Park

Department of Molecular Engineering, Kyoto University, Japan

For semiconductors in molecular optoelectronic applications, photoinduced generation and recombination dynamics of free-carriers (mobile electrons and holes) are the key process of the device operation. To probe this dynamics, various spectroscopic and electrical techniques have been utilized. In this presentation, I will discuss photoinduced carrier-dynamics probed by flash-photolysis time-resolved microwave conductivity (fp-TRMC) experiments, which are visible-pump/microwave probe spectroscopic measurements. First, my presentation will introduce free-carrier dynamics in various organic and inorganic systems studied by fp-TRMC. This study highlights the unique features of fp-TRMC such as electrode-less and non-invasive measurements and extremely high sensitivity that suppresses many-body interactions. Second, my presentation will discuss the exciton/carrier dynamics studies of complementary fp-TRMC and pump-probe transient absorption spectroscopy in solid-state organic systems where new photophysical phenomena relevant carrier-generation and recombination processes were identified.

Symposium : **PHYS3-3**

[KCS-GDCh Joint Symposium] Recent International Trends in Spectroscopic and Computational Chemistry

Room 324A, FRI 15:25

Chair: Kiyoung Park (KAIST)

Understanding elementary steps in heterogeneous (photo)catalysis

Katharina Al-Shamery

Institute of Chemistry, Carl von Ossietzky University Oldenburg, Germany

Most of the basic chemicals are produced in industry using heterogeneous catalysts. However, in order to optimize the catalysts for a specific reaction, an understanding of the underlying elementary processes is essential, but often lacking. Photocatalytic processes are even more complex. The presentation will highlight most recent findings from fundamental studies with a focus on oxidic catalysts partially modified with metal nanoparticles. Issues such as the influence of defects on the population of certain reaction pathways, strong metal support interactions (SMSI), alloying or hot electron dynamics in complex systems will be tackled. One of the focal points will be on TiO₂ as it is nontoxic, earth abundant and low priced and thus has been widely studied also in view of its interesting photocatalytic properties.^[1-6] Model reactions such as low temperature partial oxidation of methanol to formaldehyde as well as C-C-coupling of benzaldehyde will be emphasized.

References

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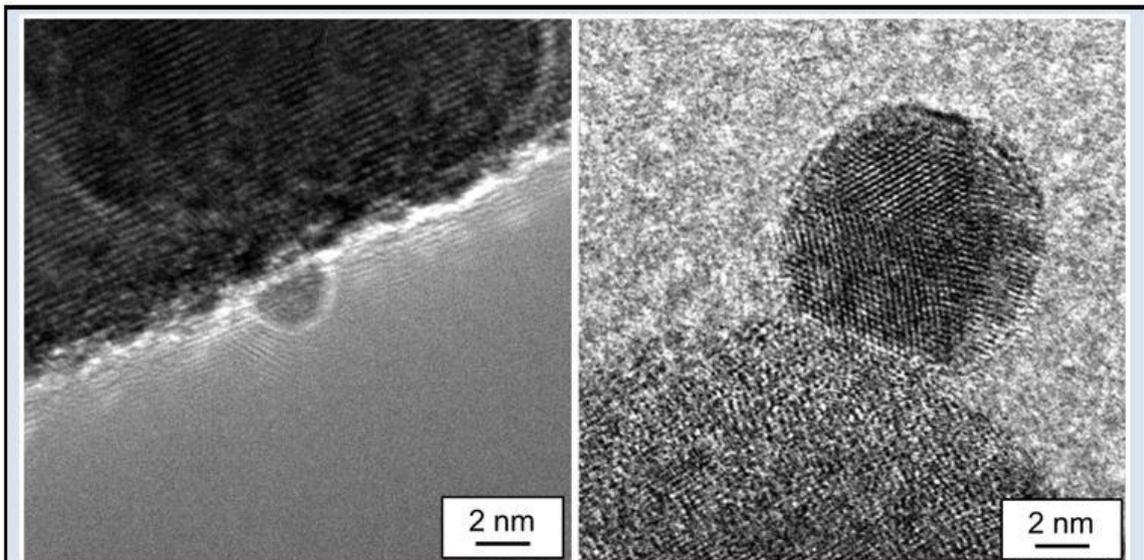


Figure: HR-TEM-studies of the Strong Metal Support Interaction (SMSI) of different metal nanoparticles capped with Oleylamine on a TiO_2 support: left: Pt; right: Au

Symposium : **PHYS3-4**

[KCS-GDCh Joint Symposium] Recent International Trends in Spectroscopic and Computational Chemistry

Room 324A, FRI 15:50

Chair: Kiyoung Park (KAIST)

Toward Understanding of Complex Solid-Liquid Interfaces

Hyungjun Kim

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

Chemistry at the interface of dissimilar materials and phases of matters is often very exotic compared to the bulk phase chemistry. In particular, solid-liquid interfaces have their own importance due to their ubiquity in a variety of applications, such as heterogeneous catalysts and electrochemical systems for sustainable energy conversion and storage. However, because of their high degree of complexity and difficulty in experimental characterizations, the molecular level of details at the solid-liquid interfaces are barely understood to date, which impedes the further development and optimization of the chemistry at the interface. In such case, theory can be the best option; however, there is no proper simulation method that can describe both phases at the full atomic level in a computationally efficient manner. We thus develop a first-principles based multiscale simulation method to understand, predict, and design the chemistry at the complex materials interface. In this talk, I will discuss our recently developed multiscale simulation method, namely a density functional theory in classical explicit solvents (DFT-CES), and demonstrate how theory and computational simulations can aid understanding the exotic chemistry at the solid-liquid interface, which can suggest a theoretical guideline for developing better materials interfaces, heterogeneous catalysts, and electrochemical systems.

Symposium : **PHYS3-5**

[KCS-GDCh Joint Symposium] Recent International Trends in Spectroscopic and Computational Chemistry

Room 324A, FRI 16:15

Chair: Kiyoung Park (KAIST)

Finding multiple reaction pathways via global optimization of action

Juyong Lee

Department of Chemistry, Kangwon National University, Korea

Global searching for reaction pathways is a long-standing challenge in computational chemistry and biology. Most existing approaches perform only local searches due to computational complexity. Here we present a computational approach, Action-CSA, to find multiple diverse reaction pathways connecting fixed initial and final states through global optimization of the Onsager–Machlup action using the conformational space annealing (CSA) method. Action-CSA successfully overcomes large energy barriers via crossovers and mutations of pathways and finds all possible pathways of small systems without initial guesses on pathways. The rank order and the transition time distribution of multiple pathways are in good agreement with those of long Langevin dynamics simulations. The lowest action folding pathway of FSD-1 is consistent with recent experiments. The results show that Action-CSA is an efficient and robust computational approach to study the multiple pathways of complex reactions and large-scale conformational changes.

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

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 17:10

Chair: Han Bin Oh (Sogang University)

Mass spectrometry of surfaces tailored with biomolecules and nanostructures, and non-covalent complexes

Sang Yun Han

Department of Nanochemistry, Gachon University, Korea

In this talk, development of mass spectrometric methods and applications that have not been in the regime of conventional mass spectrometry will be presented. (1) Mass spectrometry (MS) of surfaces tailored with biological molecules such as protein chips on which various antibodies are immobilized using self-assembled monolayers (SAMs) have been investigated as a new way of molecular diagnosis. In an effort to characterize SAMs on gold, cation-assisted laser desorption ionization (LDI) MS was developed. In the course of this study, the mechanism of MALDI for SAMs on Au was carefully elucidated. In addition, the method of microwave-assisted on-chip tryptic digestion for protein chips was further developed for rapid characterization of label-free detection of biochips. (2) Using nano-structured surfaces, the mechanism for matrix-free LDI process was investigated, which revealed rapid surface heating plays a key role in intact desorption of thermally labile molecules such as peptides. From this finding, by choosing surfaces of appropriate thermal property, LDI of large molecules was successfully demonstrated even without matrix or surface nanostructures. (3) Tandem mass spectrometry was further extended to understand intermolecular interactions such as ionic hydrogen bonding and hydrogen bonding involved in proton-bound dimers of nucleic acid bases and in G-quadruplexes. As a result, it was demonstrated that hydrogen bonding interactions that create formation of non-covalent complexes also plays an important role in determining the fate of collisionally activated complexes in dissociation. Accordingly, mass spectrometry is a powerful tool of which applications can be further extended beyond its conventional role of rapid characterization of large and complex molecules.

Award Lecture in Division : **ANAL1-6**

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 17:30

Chair: Han Bin Oh (Sogang University)

Analytical Approaches to a Failure Analysis from chemicals to devices in Displays

Hyuk Nyun Kim

Department of Analytical Technology, LG Display, Korea

The Display industries in Korea have been played important roles in the production of various displays such as LCDs and OLEDs, as a core technology based business of Korea since 2000. More advanced developments and production of better performed products of various displays from mobile to large TV applications, have always been required appropriate analytical tools or methods which can help us to monitor higher quality manufacturing and to identify the root cause of problems.

To improve the quality of state of the art display products, we need to find out and verify the failure mechanism of defects such as dark spots, bright spots, an abnormal display such as mura and image sticking as well as the mechanism of degradation of life time of OLEDs. We discuss the general analytical approaches to elucidate the root causes of display defects and decay of life time of displays using from chemical analytical instruments, GC-MS, LC-MS, SFC-MS to surface sensitive analytical instruments, XPS/ToF-SIMS/D-SIMS and structural analytical instruments, TEM/FIB/SEM with various sample pre-treatment tools for chemicals, components and devices.

Symposium : **ANALI-1**

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 15:40

Chair: Min-Sik Kim (DGIST)

Multi-dimensional Micro Gas Chromatography Device for Indoor Air Analysis

Jiwon Lee

Center for Environment, Health and Welfare, Korea Institute of Science and Technology, Korea

People routinely working with chemicals in their workplaces would be exposed to more volatile organic compounds (VOCs) and at higher concentrations than in other environments during the workdays. VOCs commonly encountered in the workplace can exert various forms of acute and chronic health effect, depending upon the particular chemical along with its exposure time and concentration. Therefore, monitoring those VOCs on-site can help ensure the safe and healthful condition and guide an immediate first aid for workers. Traditional airborne VOC on-site monitoring methods require longer sample times and an external lab, which may not provide results for several days following the exposure event. Here, a fully automated portable comprehensive 2-dimensional (2-D) gas chromatography (GC) device (60 cm × 50 cm × 10 cm and

Symposium : **ANAL1-2**

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 16:00

Chair: Min-Sik Kim (DGIST)

Introduction to Ultra-High Resolution FT-ICR Mass Spectrometry

Kyoung-Soon Jang

Biomedical Omics Center; Korea Basic Science Institute, Korea

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) has emerged as a powerful tool for the analysis of extremely complex mixtures, such as crude oils, water and soil-derived organic substances, resulting in rapid and accurate interpretation of the elemental compositions of complicated samples. The unsurpassed resolving power (full width at half maximum, FWHM: >500,000) and mass accuracy (

Symposium : **ANAL1-3**

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 16:20

Chair: Min-Sik Kim (DGIST)

Visualization of nanoparticle behavior in microchip and plant leaf using laser ablation ICP-MS

Heung Bin Lim

Department of Chemistry, Dankook University, Korea

In our lab, ICP-MS immunoassay has been developed for the detection of biomarkers in serum, which recently expanded to viruses such as HIV-1 and HBsAg. Since multiplex detection became inevitable for clinical diagnosis, microchip sampling with laser ablation (LA) was studied in this work, for this, a microchip with 8x8 pillar-type islands, 300 μm in height and 250 μm in diameter was designed. First of all, behavior of metallic ions and nanoparticles as deposited on the island was visualized by LA-ICP-MS through imaging. Similarly, the behavior of SiO_2 nanoparticles in plant leaf was also studied by a designed experimental model, which has been one of the difficulties in environmental analysis due to high background and strong interferences for $^{28}\text{Si}^+$ ion. In addition, application of triple quadrupole ICP-MS to lower interfering ions and enhance sensitivity for the detection of SiO_2 nanoparticles will be discussed in this presentation.

Symposium : **ANALI-4**

Generation Networking Symposium in Analytical Chemistry

Room 321, THU 16:40

Chair: Min-Sik Kim (DGIST)

Research and life of an analytical chemist

Gae Ho Lee

Department of Chemistry, Chungnam National University, Korea

For the past 36 years, I have conducted researches and lectures as an analytical chemist. Thank you so much for having the opportunity to educate many students with pride and reward as an analytical chemist.

I am especially grateful that many studies conducted by the analyst can directly affect people's lives. It is also very thankful that the analyst can tell the public about health, food and living habits through broadcasting and the media over the past decade.

In particular, I would like to introduce research results that can affect people's real lives through www.itbfood.net.

One example is the study of water. Seventy percent of the human body is made up of water. As we get older, the amount of water in our bodies decreases.

Water plays a key role in the body, and if it is insufficient, it can cause cancer and other chronic diseases. Water makes up the largest proportion of human composition, especially blood, brain, and tissues. It provides the most important nutrients for blood, such as calcium, magnesium, sodium, and potassium, and is the most basic substance in the immune system.

When the human body lacks water, the blood pressure becomes more concentrated and the capillaries are blocked because blood is not supplied to the capillaries when circulating. In addition, problems arise when waste materials are not properly released.

People usually breathe, sweat, urine, and excretion to get a lot of water out of the body. But now 50-60 percent of Koreans are suffering from chronic dehydration because they forgot to drink water on the pretext of being busy. The false information that 2L or 3L is said to be good for a day or that eating too much is good is being circulated on the Internet. Since drinking too much water is problematic and there is a problem with eating too little, you should eat only as much as you get out through perspiration, breathing, urine and feces.

However, each person needs different amounts, so he or she should eat more in the summer. Each individual

must immediately supplement their urine with evidence of water shortage by looking at the color of the urine for a dark yellow color. But drinking too much water is bad for your health. If you urinate more than eight times a day, or if the color of your urine becomes transparent, you should cut down on the amount of water you drink. Therefore, the amount of water each person needs must be found according to the number of urine colored (light yellow) and number of urine beams (less than eight a day).

And drink water regularly as "321 Basic Recovery Movement." "3" is a regular exercise to drink 1 cup 30 minutes before meals, "2" 2 hours after meals 1 cup after 2 hours, and "1" for 1 cup before bedtime. The amount of 1 cup water varies from about 150 to 250mL, and each person must find the amount they need by urinating and urinating. If you feel thirsty, you should take it in advance because water shortages have already occurred. Therefore, if you are exercising sweating, you should drink water before exercising. As the amount of urine, salts, water-soluble vitamins and minerals escape out of the body as the amount of urine increases, you need to take in additional vegetables, fruits and salt.

There are many different kinds of water these days. There are various kinds of water, such as mineral water, hexagonal water, medicinal alkalis, reducing water, and deep ocean water. Many people say that drinking water is the most difficult and not the best way to do it.

Water is the beginning of a basic recovery.

Symposium : **ANAL2-1**

Recent Advances of Nanobiosensor for Detection of Disease Biomarkers

Room 321, FRI 14:30

Chair: Dong-Ku Kang (Incheon National University)

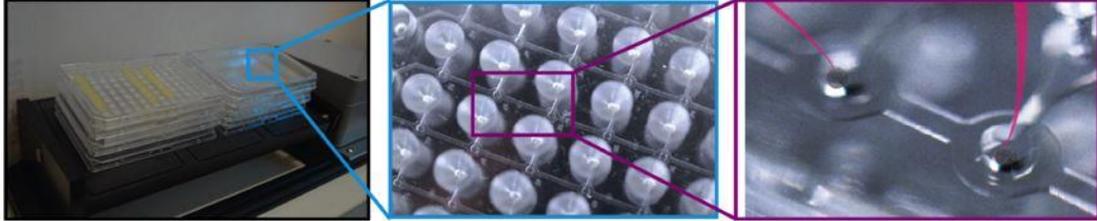
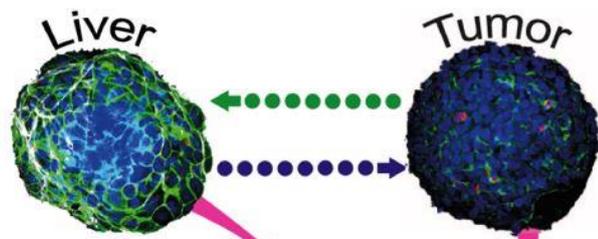
Body-on-a Chip: 3D microtissues meet microfluidics.

Jin-young Kim

DGIST-ETH Microrobotics Research Center, Daegu Gyeongbuk Institute of Science & Technology, Korea

Conventional 2D cell-based assays have limitations in mimicking *in vivo*-like environments, since multi-organ interactions, for example, side or secondary effects of metabolites produced by another organ in the body especially the liver remain obscure, are not available. Currently, such metabolic effects are only visible *in vivo*. Further, the identity, behavior, and survival of cells do not only depend on neighboring cells, but on many molecular pathways and biological processes occurring within the entire organism. In this talk, the “Body-on-a Chip” concept device is introduced, which realizes *in-vitro* multiple micro-organ network on a single device and micro-physiological fluidic condition using 3D microtissue spheroids and microfluidics. It has the potential of identifying synergistic drug interactions as well as simulating multi-organ metabolic interactions. Two-tissue configurations, here, are described with two major benefits over typical testing methods:

1. Studying not only the direct effect of compounds on an isolated target tissue alone, but also after having been metabolized by liver tissue on chip.
2. Evaluation of the efficacy of a compound on the target tissue model combined with safety and toxicity assessments on liver tissue.



Symposium : **ANAL2-2**

Recent Advances of Nanobiosensor for Detection of Disease Biomarkers

Room 321, FRI 14:50

Chair: Dong-Ku Kang (Incheon National University)

Towards Single-molecule Biosensors using Super-localization Fluorescence-free Nanoscopy

Seungah Lee, Seong Ho Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Nanoscopy based on single-molecule localization offers a practical way to explore plasmonic interactions with nanometer resolution. Over the last decade, two fields have dominated the attention of sub-diffraction photonics research: plasmonic and fluorescence nanoscopy. Fluorescence nanoscopy obstruct more sensitive and selective immunodetection due to their limitations associated with photo-stability. In contrast, plasmonic nanoscopy hold great promise for the robust quantitative nano characterization of functional nanomaterials without fluorescent labeling. We have developed high sensitive and precise nanoimmunosensors by 3D as well as 2D antibody-antigen binding on nanopatterned biochips using super-localization nanoscopy based on plasmon scattering. The biosensors have demonstrated the possibility for detection of extremely low concentration detection (i.e., μM) of various disease-related biomolecules at the single-molecule level.

Symposium : **ANAL2-3**

Recent Advances of Nanobiosensor for Detection of Disease Biomarkers

Room 321, FRI 15:10

Chair: Dong-Ku Kang (Incheon National University)

Development of redox-active ferrocene polymer for various bio-application

Daekyung Sung

*Center for Convergence Bioceramic Materials, Korea Institute of Ceramic Engineering and Technology,
Korea*

A lot of ferrocene polymers have been synthesized and used in various bio-applications. Ferrocene-containing polymers have emerged, as an important class of the metal-containing polymers, with unique redox properties and thus much considerable attention has been paid for the application of these polymer systems. The redox process may be associated with changes in the properties of the polymeric material. Thus, depending on their oxidation state (oxidized or reduced) polymers can present different electronic properties such as ionic and electrical conductivity, optical properties, mechanical or chemical properties. Due to the reversibility and easy external control of the redox process, these polymers are interesting for different applications and the design of a number of electrochemical devices such as batteries, biosensors. Furthermore, these polymers are finding new applications in materials science including the development of drug delivery systems.

Symposium : **ANAL2-4**

Recent Advances of Nanobiosensor for Detection of Disease Biomarkers

Room 321, FRI 15:40

Chair: Dong-Ku Kang (Incheon National University)

Magnetoplasmonic Nanomaterials; Synthesis, Characterization, and Biosensing Application

Jaebeom Lee

Chemistry, Chungnam National University, Korea

Nanoscale materials using plasmonic and magnetic materials have been developed to comprehend their quantum mechanical properties. A delicate assembly of the nanomaterials provided fascinating physical and optical properties. These uniqueness has been applied in the field of physical and biological sensing and imaging. In the presentation, a review including last 10 years works in the laboratory will be shown focusing on the synthesis, unique characterization, and biomedical application of magnetoplasmonic materials. A few dedication on mass production and industrialization will be also introduced.

Symposium : **ANAL2-5**

Recent Advances of Nanobiosensor for Detection of Disease Biomarkers

Room 321, FRI 16:00

Chair: Dong-Ku Kang (Incheon National University)

Structural analysis of early polyoxometalate nanoclusters using ion mobility-mass spectrometry

Jongcheol Seo

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

Advances in nanotechnology have led to the development of highly sensitive and functional nanoscale sensing materials suitable for the biomolecular detection. One of the potential candidates for such nanobiosensor materials is the polyoxometalate nanoclusters which can mediate the electrochemical potential and/or catalytic activity of specific biological process. To obtain the specific properties for biosensing applications, the three-dimensional structures and conformations of the polyoxometalate nanoclusters and their functional assemblies should be properly precisely tailored. The very first step for such structural/conformational control is to determine the structures of various polyoxometalate clusters and to understand the cluster formation mechanisms. In the present work, a new analytical approach using ion mobility-mass spectrometry was used for the structural analysis of early polyoxomolybdate clusters. Since ion mobility-mass spectrometry enables to measure the collision cross section of mass-selected individual cluster ions, the structural evolutions during the early cluster growth via pH-dependent condensation process could be monitored. The result indicates the structural transitions between 1D chain, 2D ring, and 3D compact cluster motifs as the cluster size increases. The addition of a single proton is observed to strongly influence the the adopted structure as a result of intramolecular hydrogen bonding. This is the first results which successfully analyzed the structural transitions during the polyoxomolybdate cluster growth, which clearly demonstrated that the ion mobility-mass spectrometry has great potential to analyze the structures of various nanoclusters and assemblies for further design and preparation of nanoparticle-based nanobiosensors.

Symposium : **LIFE1-1**

Structure and Function of Membrane Proteins

Room 314, THU 15:40

Chair: Hyun-Soo Cho (Yonsei University)

The functional role of Frizzled4 linker domain in Norrin signaling pathway

Hee-Jung Choi

Department of Biological Sciences, Seoul National University, Korea

Frizzled (Fzd) is a main receptor for Wnt ligand and the ligand binding to Fzd is a crucial part of Wnt signaling pathway. Published structural studies of Fzd focus on the ligand binding domain of Fzd, called cysteine-rich domain (CRD). CRD in complex with Wnt or Norrin have revealed much information on the molecular interaction between CRD and ligand. However, the question remains how that interaction with ligand is transferred across the transmembrane domain (TMD) to the intracellular region. All 10 members of Fzd family have relatively high sequence conservation in the TMD, while the extracellular and C-tail regions have low conservation. Especially of interest is the linker domain between CRD and TMD, which varies from about 40 amino acids in Fzd4 to 100 amino acid in Fzd8. Here, we show that a flexible linker domain, which connects the CRD to the TMD of Fzd4, plays an important role in Norrin signaling. The linker domain directly contributes to the high-affinity interaction between Fzd4 and Norrin as shown by ~10-fold higher binding affinity of Fzd4_{CRD} to Norrin in the presence of the linker. In addition, structural dynamics of Fzd4 associated with Norrin binding investigated by hydrogen/deuterium exchange MS revealed Norrin-induced conformational changes on the linker domain and the intracellular loop 3 (ICL3) region. Together, our results show that the linker domain plays an important role in Norrin ligand recognition, thereby its signal transmission from extracellular to intracellular regions.

Symposium : **LIFE1-2**

Structure and Function of Membrane Proteins

Room 314, THU 16:20

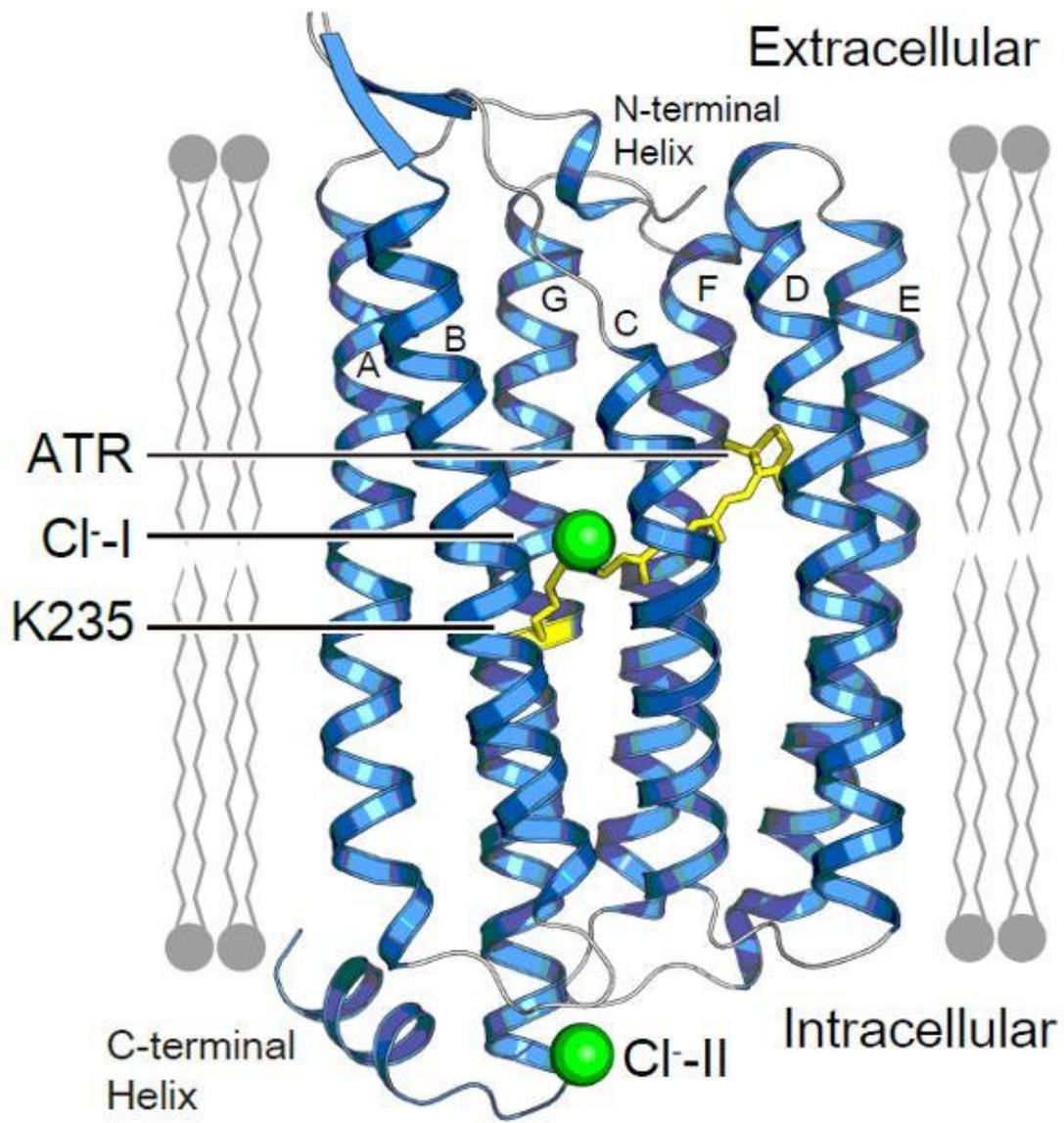
Chair: Hyun-Soo Cho (Yonsei University)

Structural analysis of a Unique Light-driven Chloride Pump Rhodopsin from marine bacteria

Hyun-Soo Cho

Yonsei University, Korea

Recently, light-driven sodium pump rhodopsin (NaR/KR2/NDQ rhodopsin) and chloride pump rhodopsin (CIR/NTQ rhodopsin) from marine flavobacteria were identified by metagenomics study. One of them, light-driven sodium pump rhodopsin (NaR) structure was determined. The other one we have solved the first crystal structure of a unique class light-driven chloride pump (CIR) from *Nonlabens marinus* S1-08, at resolutions of 1.57 Å. Like structured Halorhodopsin (HR), CIR can transfer chloride ion from extracellular to cytosol. Although both CIR and HR are same light-driven chloride pump rhodopsin, we found some evidences that CIR and HR are different in structure and mechanism. In this structure, we suggest that how chloride ion transfer from extracellular to cytosol, determine significant residues for controlling functions and confirm light-driven pump activity through mutagenesis and functional assay. Also, unlike rhodopsin family, we found that CIR has structural differences such as ECL1 and Helix 8. These results suggest that together with NaR, CIR is a unique and new molecule for optogenetic study.



Symposium : **LIFE1-3**

Structure and Function of Membrane Proteins

Room 314, THU 17:00

Chair: Hyun-Soo Cho (Yonsei University)

Structural insights into highly thermostable carbonic anhydrase for CO₂ capture and sequestration technology

Mi Sun Jin

Division of Life Science, Gwangju Institute of Science and Technology, Korea

Bacterial α -type carbonic anhydrase (α -CA) is a zinc metalloenzyme that catalyzes the reversible and extremely rapid interconversion of carbon dioxide to bicarbonate. In this study we report the first crystal structure of hyperthermostable α -CA from *Persephonella marina* EX-H1 (pmCA). The structure reveals a compact folding of the pmCA homodimer in which each monomer consists of ten-stranded β -sheet in the center surrounded by several α -helices and additional β -strands in the periphery. Catalytic zinc ion is coordinated by highly conserved residues of three histidines and a bicarbonate. Extensive intermolecular network by hydrogen bonds, ionic and hydrophobic interactions might significantly confer a high pH and thermal stability to the pmCA. Furthermore, an intramolecular disulfide bond gives an additional stabilization of the pmCA structure. We also present the first demonstration of novel binding sites for five calcium ions at the crystallographic interface, serving as a molecular glue to link the negatively charged otherwise repulsive surfaces. The data obtained in this study offer essential information that can be exploited to engineer α -CAs in order to obtain enzymes with improved thermostability for high tolerance to the harsh conditions of the CO₂ capture and sequestration technology.

Symposium : **LIFE2-1**

Recent Trends in Genome Editing Technique

Room 314, FRI 09:00

Chair: Chonsaeng Kim (KRICT)

Genome editing using CRISPR-Cas system

Sangsu Bae

Department of Chemistry, Hanyang University, Korea

Genome editing with engineered nucleases such as ZFNs (zinc finger nucleases), TALENs (transcription-activator-like effector nucleases), and CRISPR-Cas9/Cpf1 derived RNA-guided endonucleases is broadly used for biomedical research, biotechnology, and medicine. In addition, CRISPR base editors that enable the direct conversion of DNA bases without producing double-stranded breaks (DSBs) of DNA were developed. Unlike ZFNs and TALENs whose DNA specificities are determined by DNA-binding proteins, CRISPR nucleases use complementary base pairing to recognize target sites. Now, CRISPR nucleases are widely exploited due to the ease of use and inexpensive cost; researchers can induce gene editing at different sites by simply altering the guide RNAs. However, CRISPR nucleases cleave not only on-target sites but also off-target sites that differ by up to several nucleotides from the on-target sites, causing unwanted off-target mutations and chromosomal rearrangements. Here I present web-based programs, named CRISPR RGEN Tools (www.rgenome.net), including a novel CRISPR design tool and a genome editing assessment tool. These tools are indispensable for gene mutation in human cells, animals and plants. Furthermore, I would like to introduce versatile applications of CRISPR nucleases such as a one-step transformation of *Chlamydomonas reinhardtii* by the DNA-free CRISPR, a circulating tumor DNA detection and the detailed mechanism of Cas9/Cpf1 revealed by single-molecule fluorescence imaging.

Symposium : **LIFE2-2**

Recent Trends in Genome Editing Technique

Room 314, FRI 09:25

Chair: Sangsu Bae (Hanyang University)

CRISPR screening identifies host factors essential for viral infection

Chonsaeng Kim

*Center for Convergent Research of Emerging Virus Infection, Korea Research Institute of Chemical
Technology, Korea*

Pooled CRISPR screens based on lentiviral systems have been widely applied to identify the effect of gene knockout on cellular phenotype. Although many screens were successful, they also have the limitation that genes conferring mild phenotypes or those essential for growth can be overlooked as every genetic perturbation is incorporated in the same population. Arrayed screens, on the other hand, incorporate a single genetic perturbation in each well, and could overcome these limitations. However, arrayed screens based on siRNA-mediated knockdown were recently criticized for low reproducibility caused by incomplete inhibition of gene expression. To overcome these limitations, we developed a novel arrayed CRISPR screen based on a plasmid library expressing a single guide RNA (sgRNA) and disrupted 1,514 genes, encoding kinases, proteins related to endocytosis, and Golgi-localized proteins, individually using 4,542 sgRNAs (3 sgRNAs per gene). This screen revealed host factors required for infection by coxsackievirus B3 (CVB3) from Picornaviridae, which includes human pathogens causing diverse diseases. Many host factors that had been overlooked in a conventional pooled screen were identified for CVB3 infection, including entry-related factors, translational initiation factors, and several replication factors with different functions, demonstrating the advantage of the arrayed screen. This screen was quite reliable and reproducible, as most genes identified in the primary screen were confirmed in secondary screens. Moreover, ACBD3, whose phenotype was not affected by siRNA-mediated knockdown, was reliably identified. We propose that arrayed CRISPR screens based on sgRNA plasmid libraries are powerful tools for arrayed genetic screening and applicable to larger-scale screens.

Symposium : LIFE2-3

Recent Trends in Genome Editing Technique

Room 314, FRI 09:50

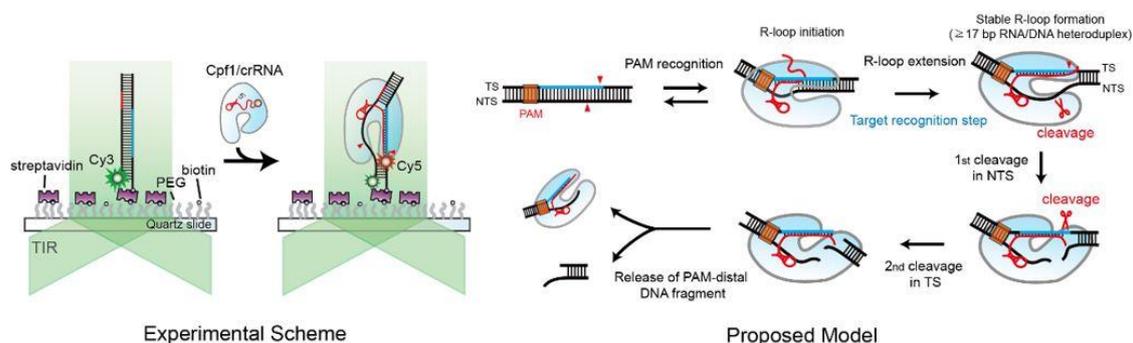
Chair: Sangsu Bae (Hanyang University)

Single-molecule FRET study on CRISPR-Cas12a endonuclease

Sanghwa Lee

Advanced Photonics Research Institute, Gwangju Institute of Science and Technology, Korea

Cas12a (also called Cpf1) is a representative type V-A CRISPR effector RNA-guided DNA endonuclease, which provides an alternative to type II CRISPR–Cas9 for genome editing. Previous studies have revealed that Cas12a has unique features distinct from Cas9, but the detailed mechanisms of DNA target recognition and cleavage by Cas12a are still unclear. In this work, we directly observe this entire process by using single-molecule fluorescence assays to study Cas12a from *Acidaminococcus* sp. (*AsCas12a*). Our results reveal that a stable R-loop formation, which is the main determinant of target recognition, is efficiently established only when the seed matches up to 17 base pairs, and *AsCas12a* ribonucleoproteins induce cleavage in the two DNA strands in a well-defined order, beginning with the non-target strand. Furthermore, the protospacer-adjacent motif (PAM) for *AsCas12a* makes only a limited contribution of DNA unwinding during R-loop formation and shows a negligible role in the process of DNA cleavage, in contrast to the Cas9 PAM.



Symposium : **LIFE2-4**

Recent Trends in Genome Editing Technique

Room 314, FRI 10:15

Chair: Sangsu Bae (Hanyang University)

Development of multi-functional guide RNA for gene manipulation using Cas9 and Cpf1

Yongsub Kim

*Department of Biomedical Sciences, University of Ulsan College of Medicine, ASAN Medical Center,
Korea*

Engineered nucleases that allow targeted mutagenesis in living cells and organisms are broadly useful in biological research. Engineered nucleases induce target specific DNA double-strand breaks (DSBs) and DSBs subsequently recruit intracellular machinery for either non-homologous end-joining (NHEJ) or homology-directed repair (HDR) to the DSB site to mediate genome editing. We have developed ZFNs, TALENs, CRISPR-mediated Cas9 and Cpf1 to modify chromosomal DNA in living cells. Using these engineered nucleases, we also generated several knockout cell lines and model organisms with high efficiencies. Also, we have developed guide RNA variants for multiplex genome engineering & orthogonal gene manipulation. These constructs will expand the use of genome editing tools in biomedical research.

Symposium : **LIFE2-5**

Recent Trends in Genome Editing Technique

Room 314, FRI 10:40

Chair: Sangsu Bae (Hanyang University)

Structures and interactions of anti-CRISPR proteins

Euiyoung Bae

Department of Agricultural Biotechnology, Seoul National University, Korea

Clustered regularly interspaced short palindromic repeats (CRISPRs) and CRISPR-associated (Cas) proteins provide bacterial adaptive immunity against bacteriophage infection. To counteract this defense mechanism, bacteriophages evolved anti-CRISPR (Acr) proteins that inactivate the anti-phage CRISPR-Cas systems. Here, we report the crystal structures of two Acr proteins, AcrF2 and AcrIIA1. AcrF2 inhibits the type I-F CRISPR-Cas system in *Pseudomonas aeruginosa*. In this type, multiple Cas proteins (Csy1-4) comprise a surveillance complex (Csy complex) with CRISPR RNA (crRNA) for target recognition. AcrF2 binds to the Csy1-Csy2 heterodimers with nanomolar affinity. In the crystal structure of AcrF2, the arrangement of carboxyl side chains resembles the negative charge distribution of the dsDNA backbone, confirming that AcrF2 is a double-stranded DNA mimic blocking target recognition. AcrIIA1, encoded by *Listeria monocytogenes* prophages, is the most prevalent among the Acr proteins targeting type II-A CRISPR-Cas systems. AcrIIA1 forms a dimer with a novel two-helical-domain architecture. The N-terminal domain of AcrIIA1 exhibits a helix-turn-helix motif similar to transcriptional factors. When overexpressed in *Escherichia coli*, AcrIIA1 associates with RNAs, suggesting that AcrIIA1 functions via nucleic acid recognition. Taken together, the structural and functional features of AcrF2 and AcrIIA1 suggest their distinct modes of Acr activity, expanding the diversity of the inhibitory mechanisms employed by Acr proteins.

Symposium : **LIFE3-1**

Exosome: from Concept to Clinic

Room 314, FRI 14:30

Chair: Kwang Pyo Kim (Kyung Hee University)

Extracellular vesicles, exosomes and mimetic technology: from bench to clinic

Yong Song Gho

Department of Life Sciences, Pohang University of Science and Technology, Korea

Throughout evolution, both prokaryotic and eukaryotic cells have adapted to manipulate extracellular vesicles for intercellular communication via outer membrane vesicles in the case of Gram-negative bacteria and exosomes or ectosomes (also known as microvesicles) or in eukaryotic cells. Extracellular vesicles play multiple roles in intercellular and interspecies communication, suggesting that extracellular vesicles are NanoCosmos (<http://evpedia.info>). This presentation focuses on the comprehensive aspects of mammalian and bacterial exosomes including components, biogenesis, and diverse functions that should facilitate further applications, especially to develop therapeutics including our recent progress in novel exosome-mimetic technology for targeted drug and vaccine delivery platforms and for tissue regeneration. Future research and business directions of Rosetta Exosomes (<http://www.rosettaexosome.com>) to isolate and characterize the exosomes for basic researches and clinical applications will be briefly introduced.

Symposium : **LIFE3-2**

Exosome: from Concept to Clinic

Room 314, FRI 15:00

Chair: Kwang Pyo Kim (Kyung Hee University)

Extracellular vesicles as a platform for membrane-associated therapeutic protein delivery

Yoosoo Yang

Korea Institute of Science and Technology, Korea

Membrane proteins are of great research interest, particularly because they are rich in targets for therapeutic application. The suitability of various membrane proteins as targets for therapeutic formulations, such as drugs or antibodies, has been studied in preclinical and clinical studies. For therapeutic application, however, a protein must be expressed and purified in as close to its native conformation as possible. This has proven difficult for membrane proteins, as their native conformation requires the association with an appropriate cellular membrane. One solution to this problem is to use extracellular vesicles as a display platform. Exosomes and microvesicles are membranous extracellular vesicles that are released from most cells. Their membranes may provide a favourable microenvironment for membrane proteins to take on their proper conformation, activity, and membrane distribution; moreover, membrane proteins can cluster into microdomains on the surface of extracellular vesicles following their biogenesis. In this review, we survey the state-of-the-art of extracellular vesicle (exosome and small-sized microvesicle)-based therapeutics, evaluate the current biological understanding of these formulations, and forecast the technical advances that will be needed to continue driving the development of membrane protein therapeutics.

Symposium : **LIFE3-3**

Exosome: from Concept to Clinic

Room 314, FRI 15:20

Chair: Kwang Pyo Kim (Kyung Hee University)

Harnessing Intercellular Transfer of Exosomes to Improve Drug Delivery

Ji Ho Park

Bio and Brain Engineering, KAIST, Korea

Over the past decade, widespread progress in nanotechnology has produced an impressive array of nanodevices with powerful therapeutic properties. Nonetheless, our capacity to precisely home these devices to regions of disease in vivo has remained very limited and, despite three decades of research, ligand-targeted nanomedicines have yet to provide a benefit to patients. A fundamental limitation of current approaches to nanomedicine delivery is that they lack capabilities of tissue penetration of therapeutic agents. In this talk, I will introduce our recent approaches to leveraging biological nanoparticles to improve drug delivery. We have developed a series of drug delivery nanosystems where extracellular vesicles in the tumor microenvironment were engineered in situ to improve tumor penetration of functional and therapeutic compounds and the therapeutic efficacy.

Symposium : **LIFE3-4**

Exosome: from Concept to Clinic

Room 314, FRI 15:40

Chair: Kwang Pyo Kim (Kyung Hee University)

Isolation and Analysis of Extracellular Vesicles

Jaesung Park

Mechanical Engineering/ I-Bio, Pohang University of Science and Technology, Korea

In research about extracellular vesicles, two limitations hinder advances, isolation and analysis of extracellular vesicles. For better isolation, we adapted the aqueous two-phase system (ATPS) to diagnose prostate cancer by isolating EVs from patients' urine. ATPS was optimized by adjusting polymer concentration. EVs were isolated in the first phase with efficiency of ~100%; total processing time is just ~ 30 min. After the ATPS isolated EVs from patients' urine, PCR and ELISA kit were used to detect EVs derived from prostate cancer cells. The expression levels of mRNA and protein markers of prostate cancer were measured, and the relationship between expression levels and clinical data was analyzed. As a result, diagnostic ability based on ATPS is better than conventional ones (serum PSA and sediments); sensitivity is increased at least 10%, and specificity is improved at least 20% compared to conventional methods

Along with isolation, analysis of extracellular vesicle is challenging as well. For analysis of heterogeneity of extracellular vesicles, the multi-color particle tracking analysis system for quantified characterization of individual extracellular vesicles is developed, which simultaneously analyzes trajectories of multiple suspended particles visualized by scattered light and fluorescence of three colors. The fluorescence particle test shows that the algorithm showed 0.22% false positives and 8.3% false negatives for the fluorescence signal. This system is capable of tracking the signal of SYTO nucleic acid dye stained inside EV and fluorescence protein expressed in EV as well as bright dye. Using various combinations of fluorescence staining, it is possible to distinguish subpopulation of particles bearing each marker in the human plasma. Through the subpopulation, it is estimated the number of total particle, particles bearing genes, lipoproteins and particles bearing extracellular vesicle (EV) related markers. Also, the colocalization of fluorescent probes is analyzed to determine the tendency of which markers are likely to coexist in the same particle. By combing those methods mentioned above , we could analyze subpopulation of extracellular vesicles, and could be useful in diagnosis, extracellular vesicle quality control in therapeutic applications.

Symposium : **LIFE3-5**

Exosome: from Concept to Clinic

Room 314, FRI 16:00

Chair: Kwang Pyo Kim (Kyung Hee University)

Clinical application of stem cell-derived EV-therapy

Oh Young Bang

Neurology, Samsung Medical Center, Korea

Stem cell therapy is the promising therapeutic strategies for human diseases with no curable treatment option. Extracellular vesicles (EVs) are defined as a heterogeneous population of small vesicles with a diameter of 0.1 to 1 μm . Beside the role of EVs in the biomarker research field, it has been identified that EVs have their own therapeutic functions: EVs play a critical role in the exchange of information between cells. For examples, EVs secreted from mesenchymal stem cells (MSCs) alter the behavior of the target cells and promote restorative processes. Recently, there have been advances in terms of modification of stem cell-derived EVs to enhance their functions and the methods for isolation and production of EVs. However, there exist several hurdles in the application of EVs in humans, and only few clinical trials was conducted in clinical trials. In this talk, the recent advances of stem cell-derived EV-based therapies, including their potential benefits and underlying mechanisms, will be discussed together with the current limitations in the application in human.

Award Lecture in Division : **ORGN1-1**

[KCS-GDCh Joint Symposium] Current Trends in Organic Chemistry I: Total Synthesis and Synthetic Methods
Development

Room 325A+B, THU 15:40

Chair: Young Ho Rhee (POSTECH)

Function-driven Design and Synthesis of Organic Molecules: From Optoelectronic Materials to Functional Polymers

Bongjin Moon

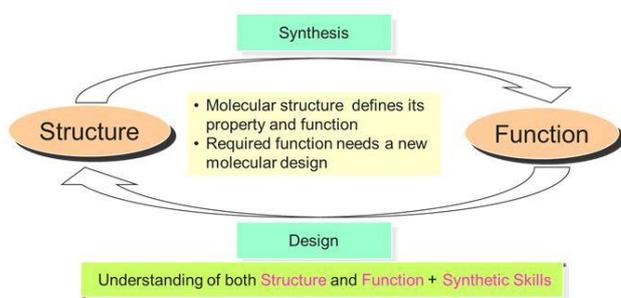
Department of Chemistry, Sogang University, Korea

As the need for sophisticated functional materials expands, expertise in synthetic organic chemistry has become more pivotal in developing new functional materials from the early designing-stage. In contrast to the traditional target-oriented organic synthesis which generally starts with a given target compound structure, function-driven organic synthesis should begin with understanding of the desired function of the materials to be synthesized. In depth understanding of the function as an organic chemist then enable him or her to design new molecules with optimal synthetic pathways. Over the last 16 years, our lab has been interested in developing new organic materials that exhibit interactions with three non-chemical stimuli; electricity, light, and heat. Electrochromic and conducting polymers are some of the examples for the electroactive organic materials studied in our lab.¹ Taking advantage of modern polymerization techniques such as controlled free radical polymerization (ATRP, NMRP, RAFT) and living ring opening metathesis polymerization (ROMP) along with wisely selected synthetic strategies, we could design and synthesize organic materials with finely tuned and desirable functionalities. Some examples include photocleavable block copolymer,² thermally activable ketene-generating polymers,³ MS tags for free radical initiated peptide sequencing (FRIPS),⁴ and matrix-free MS tags for laser desorption ionization (LDI).⁵ In this talk, a review of the research efforts made in our lab in these fields will be provided.

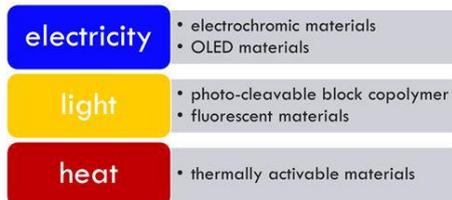
References

1. (a) Ko, H. C.; Kang, M.; Moon, B.; Lee, H. *Adv. Mater.* **2004**, 16, 1712. (b) Ko, H. C.; Kim, S.; Lee, H.; Moon, B. *Adv. Funct. Mater.* **2005**, 15, 905. (c) Park, Y. S.; Kim, D.; Lee, H.; Moon, B. *Org. Lett.* **2006**, 8, 4699. (d) Heo, G.; Moon, B. *Tetrahedron Lett.* **2008**, 49, 5540. (e) Kim, S.-H.; Shim, N.; Lee, H.; Moon, B. *J. Mater. Chem.* **2012**, 22, 13558.
2. Kang, M.; Moon, B. *Macromolecules* **2009**, 42, 455.

3. (a) Leibfarth, F.; Kang, M.; Ham, M.; Kim, J.; Campos, L. M.; Gupta, N.; Moon, B.; Hawker, C. J. *Nature Chem.* **2010**, 2, 207. (b) Leibfarth, F. A.; Schneider, Y.; Lynd, N. A.; Schultz, A.; Moon, B.; Kramer, E. J.; Bazan, G. C.; Hawker, C. J. *J. Am. Chem. Soc.* **2010**, 132, 14706.
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5. Kang, N.; Lee, J.-M.; Jeon, A.; Oh, H. B.; Moon, B. *Tetrahedron* **2016**, 72, 5612.



Developing new materials that are responsive to *non-chemical stimuli*



Symposium : **ORGN1-2**

[KCS-GDCh Joint Symposium] Current Trends in Organic Chemistry I: Total Synthesis and Synthetic Methods
Development

Room 325A+B, THU 16:10

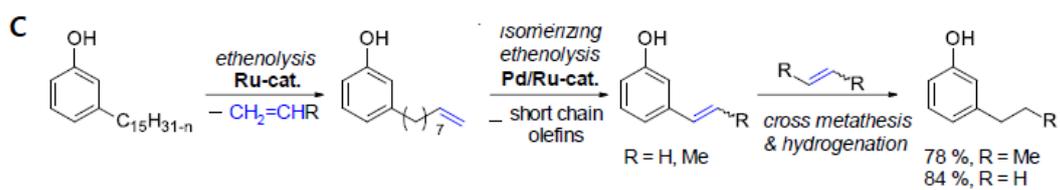
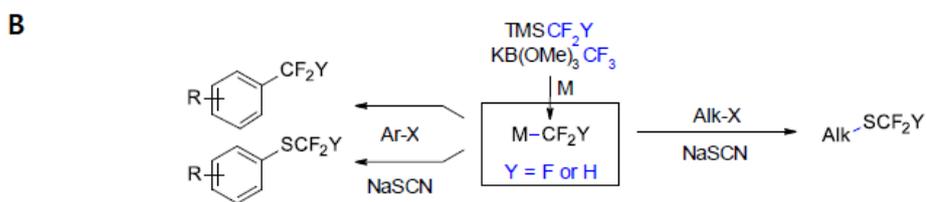
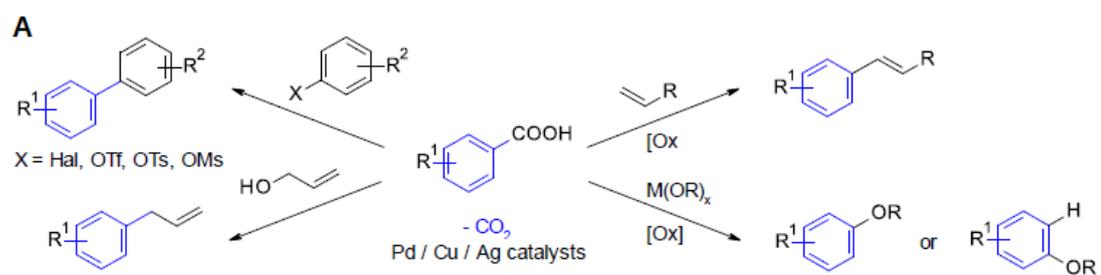
Chair: Sunkyu Han (KAIST)

Inventing Reactions - Catalytic activation of C-C, C-O, C-N, and C-H bonds

Lukas Gooßen

Chemistry and Biochemistry, Ruhr-Universität Bochum, Germany

Since our initial report in 2006, decarboxylative coupling reactions, i.e. reactions in which C–C bonds to carboxylate groups are cleaved with formation of new carbon–carbon bonds, have evolved into a powerful synthetic strategy. Their key benefit is that they draw on easily available carboxylic acids rather than expensive organometallic reagents as sources of carbon nucleophiles. Decarboxylative couplings have been utilized e.g. in syntheses of biaryls, vinyl arenes, aryl ketones and aryl ethers. The decarboxylative Chan-Evans-Lam alkoxylation of benzoic acids demonstrates that this reaction concept is applicable also to C–heteroatom bond-forming reactions. In recent variations of this reaction type, the carboxylate groups are first utilized as directing groups for ortho-C–H functionalizations and then either cleaved tracelessly or used as leaving groups in subsequent ipso-substitution reactions. In such transformations, the arene substitution pattern of the benzoate substrates is altered in a defined way, so that they ideally complement the preceding protocols. Besides decarboxylative couplings, other sustainable C–C and C–heteroatom bond-forming concepts will be discussed including fluoroalkylations and isomerizing olefin metatheses. References (a) L. J. Gooßen, G. Deng, L. M. Levy, *Science* 2006, 313, 662–664. (b) S. Bhadra, W. I. Dzik, L. J. Gooßen, *Angew. Chem. Int. Ed.* 2013, 52, 2959–2962. (c) B. Bayarmagnai, C. Matheis, K. Jouvin, L. J. Gooßen, *Angew. Chem.* 2015, 127, 5845–5848. (d) L. Huang, A. Biafora, G. Zhang, V. Bragoni, L. J. Gooßen, *Angew. Chem. Int. Ed.* 2016, 55, 6933–6937. (e) K. F. Pfister, S. Bader, M. Baader, S. Berndt, L. J. Goossen, *Sci. Adv.* 2017, 3, e1602624. (f) X.-Q. Hu, Z. Hu, A. S. Trita, G. Zhang, L. J. Gooßen, *Chem. Sci.* 2018, 9, 5289–5294.



Symposium : **ORGN1-3**

[KCS-GDCh Joint Symposium] Current Trends in Organic Chemistry I: Total Synthesis and Synthetic Methods
Development

Room 325A+B, THU 16:40

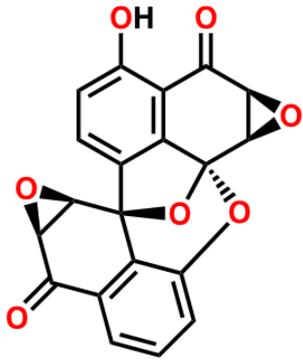
Chair: Sunkyu Han (KAIST)

Lessons from Total Synthesis of Complex Natural Products

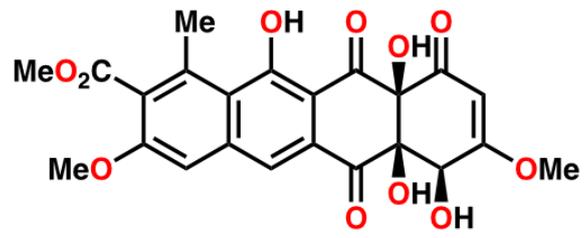
Keisuke Suzuki

Chemistry, Tokyo Institute of Technology, Japan

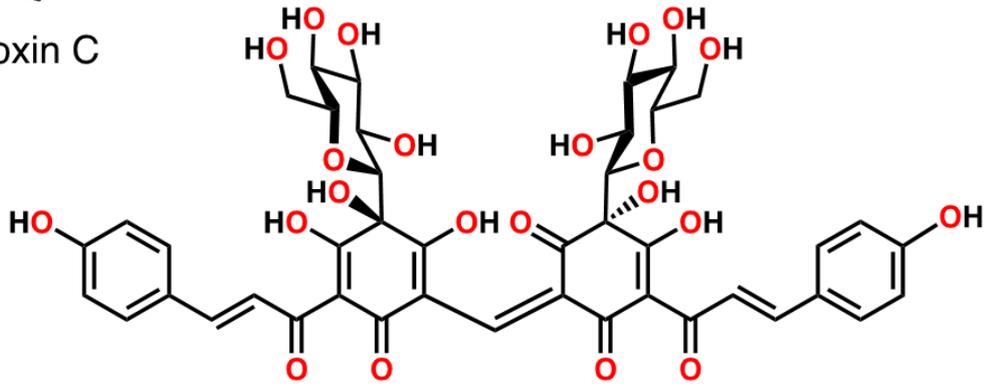
Enchanted by the structural beauty and diversity, we have been engaged in the research on total synthesis of complex natural products. Particularly, we focused attention to the natural products derived from the type-II polyketide biosynthesis, which is as a remarkable pathway, generating an impressive array of compounds characterized by densely functionalized polycyclic architectures with various significant biological activities. The biosynthetic process starts with multiple Claisen condensations of acetate units to generate skipped polyketones, and folding within an enzyme pocket and repeated aldol condensations generate nascent polycycles. Differences in the polyketide chain length as well as the mode of folding provide substantial level of molecular diversity. In addition, the diversity is further enhanced by (1) the post modifications, including oxidative de-aromatization, (2) the dimerization or oligomerization, and (3) the hybridization with other biosynthetic products, such as sugars and/or isoprenoids. This talk will deal with some recent findings made in the synthesis of three natural products.^{1,2,3,4}References 1) Suzuki, K. *Chem. Rec.*, 2010, 10, 291. 2)(a) Hayashi, D.; Ohmori, K.; Suzuki, K. *Synlett*, 2016, 27, 2345. (b) Hayashi, D.; Ohmori, K.; Suzuki, K. *Org. Lett.*, 2017, 19, 866. 3) Ando, Y.; Sasaki, Y.; Ohmori, K.; Suzuki, K. *Angew. Chem. Int. Ed.*, 2017, 56, 11460. 4) Sato, S.; Sakata, K.; Hashimoto, Y.; Takikawa, H.; Suzuki, K. *Angew. Chem. Int. Ed.*, 2017, 56, 12608.



spiroxin C



tetracenomycin C



carthamin

Symposium : **ORGN1-4**

[KCS-GDCh Joint Symposium] Current Trends in Organic Chemistry I: Total Synthesis and Synthetic Methods
Development

Room 325A+B, THU 17:20

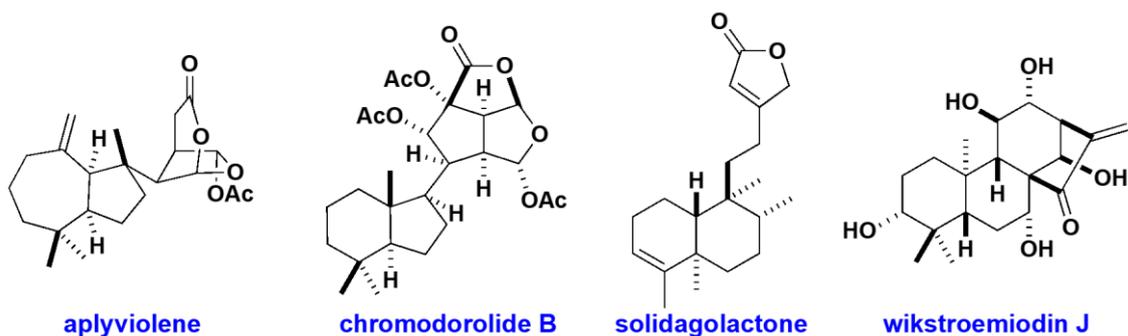
Chair: Sunkyu Han (KAIST)

Fragment Coupling with Carbon Radicals

Larry E. Overman

Chemistry, University of California, Irvine, United States

Reactions that allow complex molecular fragments to be combined in high yield occupy an exalted position in organic synthesis because they are fundamental to convergent synthesis strategies. Recent discoveries from our laboratories show that bimolecular reactions of structurally elaborate tertiary carbon radicals and electron-deficient alkenes can unite complex fragments by forming a new sp^3 - sp^3 in good yield using equimolar amounts of the two coupling partners. Reflecting the large steric bulk of tertiary carbon radicals, these reactions can take place with high stereoselectivity to form new quaternary and tertiary carbon stereocenters. Tertiary carbon radicals are generated conveniently using visible-light photocatalysis, which offers distinct advantages over older, less-green, methods for forming carbon radicals.



Symposium : **ORGN2-1**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 325A+B, FRI 09:00

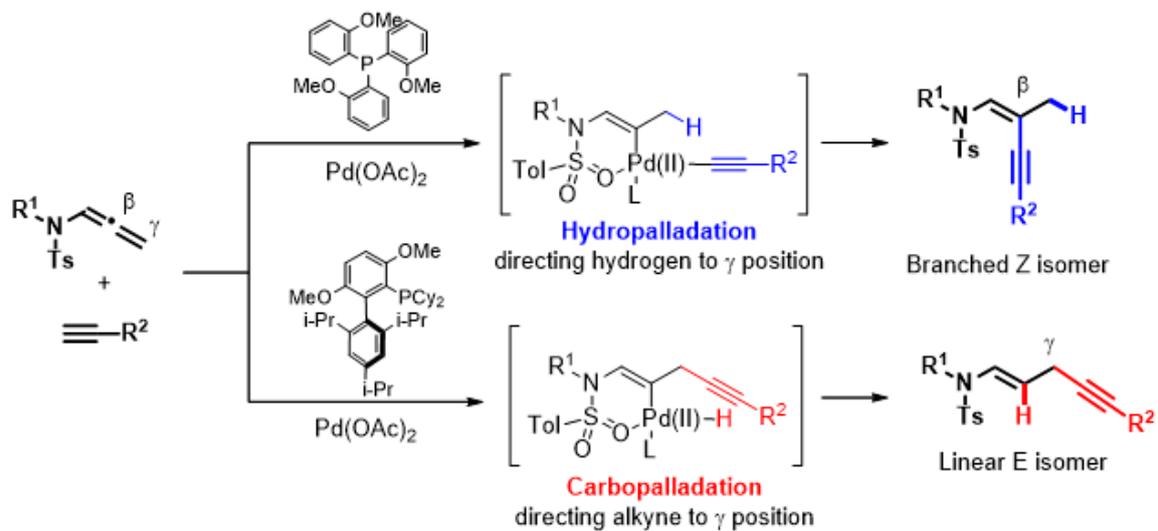
Chair: Seewon Joung (Mokpo National University)

Ligand-enforced Carbopalladation and Kinetically Favored Hydropalladation Leading to Skipped- and Conjugated Enynes

Jin Kyoon Park

Department of Chemistry, Pusan National University, Korea

An examination of the previously reported palladium-catalyzed hydroalkynylation of allenes revealed that there exist a common trans geometry and conjugated branch selectivity (β -alkynylation) for neutral and electron-deficient allenes, presumably governed by the thermodynamic stability of the product. The β -alkynylation proceeds via the formation of π -allyl-Pd intermediate through carbopalladation pathway. Given this known propensity of allenes, the possibility of divergent β - and γ -alkynylation stood as a challenging and unprecedented task. In order to address this challenge, we attempted to take advantage of the potential chelating amide group of the substrate for control of the stereoselectivity and to screen sterically and electronically differentiated phosphine ligands for the desired regiocontrol. Herein, we present a complementary, highly regiodivergent, and stereospecific cross-coupling approach for the syntheses of conjugated and skipped ynamides promoted by two different ligands, using a single metal catalyst (Figure). We also proposed reasonable mechanisms in which the hydro- and carbopalladation processes in the current divergent reaction operate separately by the formation of σ -vinyl-Pd intermediate, based upon experimental results.



Symposium : **ORGN2-2**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 325A+B, FRI 09:25

Chair: Seewon Joung (Mokpo National University)

Visible-light-induced radical reactions: Applications in the synthesis of bioactive molecules

Anna Lee

Department of Chemistry, Myongji University, Korea

Recently, visible-light-mediated photoredox catalysis has emerged as a powerful tool in organic synthesis.¹ Transition metal-based photocatalysts such as ruthenium and iridium polypyridyl complexes are widely employed in photoredox catalysis with great reported success. However, based on the limitations of utilizing transition metals, the development of green activation modes in photoredox system is very important. In this presentation, I will present recent work on organo-photocatalysis and photocatalyst-free reactions and their applications in the synthesis of bioactive molecules.² 1. (a) K. Zeitler, *Angew. Chem. Int. Ed.* **2009**, *48*, 9785. (b) T. P. Yoon; M. A. Ischay; J. Du, *Nature Chem.* **2010**, *2*, 527. (c) J. M. R. Narayanam; C.R. J. Stephenson, *Chem. Soc. Rev.* **2011**, *40*, 102. (d) L. Shi; W. Xia, *Chem. Soc. Rev.* **2012**, *41*, 7687. (e) J. W. Tucker; C. R. J. Stephenson, *J. Org. Chem.* **2012**, *77*, 1617. 2. (a) B. Hong; J. Lee; A. Lee, *Tetrahedron Lett.* **2017**, *58*, 2809. (b) D. H. Kim; J. Lee; A. Lee, *Org. Lett.* **2018**, *20*, 764.

Symposium : **ORGN2-3**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 325A+B, FRI 10:00

Chair: Min Kim (Chungbuk National University)

Mechanochemical Macromolecule Synthesis

Jeung Gon Kim

Department of Chemistry, Chonbuk National University, Korea

Mechanochemical reactions, chemical reactions those are induced by the direct absorption of mechanical energy, are promising methods to break and form chemical bonds. Beyond an alternative to thermo-, photo-, or electrochemical activation methods, mechanical-force-driven chemical synthesis can show unexpected reactivity and selectivity, which conventional approaches cannot achieve. Moreover, the exclusion of solvents reduces a processing cost and minimizes the environmental effects. While many areas of chemistry have enjoyed the merits of mechanochemistry, it has been unexplored in polymer synthesis. Applying mechanical stress on polymeric materials has been regarded to cause degradation. Recently, we stated to pursue the use of mechanical force for the construction of macromolecules and a mechanochemical polymerization of lactide is developed using ball milling. Mechanical energy from the collisions between the balls and the vessel efficiently promoted an organic-base-catalyzed metal- and solvent-free solid-state polymerization. Also solid-state post-polymerization modification was achieved by means of mechanochemistry as well. The current status of mechanochemical polymer synthesis by our research team will be presented.

Symposium : **ORGN2-4**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 325A+B, FRI 10:25

Chair: Min Kim (Chungbuk National University)

Efficient Synthetic Methods using Benzyne for Bioactive molecules

Haye Min Ko

Department of Bio-nanochemistry, Wonkwang University, Korea

The 1-ethyl-4-phenylpiperazine motif plays an important role and is an essential structure in many compounds used in a variety of fields, such as material, agrochemical, and medicinal chemistry. Especially, bioactive molecules having these privileged heterocycles have found widespread applications as drug candidates or experimental drugs. 2-(4-Phenylpiperazin-1-yl)ethyl-containing derivatives are known to possess several bioactivities such as antitumor, antiinflammatory, antiobesity, and cardiovascular activities. Despite their potential and usefulness, methods to construct this scaffold have been extremely limited. To overcome the synthetic difficulty and limitation of structural diversity, we focused our attention on aryne-mediated three-component reactions under transition-metal-free conditions. In particular, benzyne, which can be generated from *o*-silyl aryl triflates, are very reactive intermediates owing to a strained π -bond. However, to the best of our knowledge, extensive research of this reaction using DABCO to obtain 1-ethyl-4-phenylpiperazine-containing derivatives has not been sufficiently explored. Therefore, we decided to examine the reaction of tertiary amines, such as *N*-methyl morpholine or DABCO with arynes. References 1) J. H. Seo, H. M. Ko, *Tetrahedron Lett.* 2018, 59, 671-6742) G. Min, J. Seo, H. M. Ko, *J. Org. Chem.* 2018, 83, 8417-8425

Symposium : **ORGN3-1**

[Korea-Poland Joint Organic Chemistry Symposium] Recent Advances in Organic Chemistry in Cognate Areas of
Biology and Materials

Room 325A+B, FRI 14:30

Chair: Hee-Seung Lee (KAIST)

Conformationally rigid, β,β' -fused antiaromatic hexaphyrins[1.0.1.0.1.0]: structure and redox properties

Chang Hee Lee

Department of Chemistry, Kangwon National University, Korea

A β,β' -fused, (1.0.1.0.1.0)hexaphyrin derivatives are Huckel's $4n\pi$ anti-aromatic system. The compounds are known to form stable $(4n+1)\pi$ dication radical species upon exposure to acids. Naphthosarin derivatives especially bearing substituents on the periphery were not reported due to the limited accessibility to the key building blocks. We have been interested in developing a generic synthetic pathway to the key building blocks that can lead to the peripherally substituted, new naphthosarins. As the results, we successfully synthesized several new naphthosarins building blocks and corresponding naphthosarins. The structural and spectroscopic properties, redox properties and protonation behavior was studied. The results revealed interesting chemistry. The redox properties and protonation behavior of the newly synthesized naphthosarins was studied. The absorption spectral changes after addition of acids indicates that the single electron reduction rates vary depending on the peripheral substituents. Slightly increased reduction potential of substituted rosarin and the electron withdrawing nature of fluoride exhibited dramatically different redox properties. The findings clearly indicate that the fine-tuning of the redox properties is possible by introduction of various peripheral substituents.

Symposium : **ORGN3-2**

[Korea-Poland Joint Organic Chemistry Symposium] Recent Advances in Organic Chemistry in Cognate Areas of
Biology and Materials

Room 325A+B, FRI 14:55

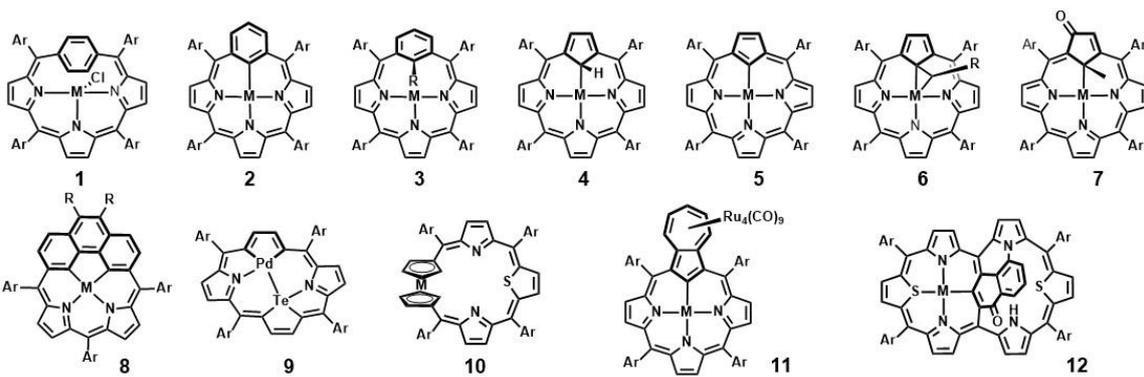
Chair: Hee-Seung Lee (KAIST)

Carbaporphyrinoids – A Quest for Flexible Macrocyclic Surroundings in Organometallic Chemistry

Lechoslaw Latos-Grazynski

Chemistry, University of Wroclaw, Poland

Redesign of archetypical porphyrin frame, introducing of CH unit(s) in place of one of the pyrrolic nitrogen atoms, created an original class of macrocycles - carbaporphyrinoids, which reveal fascinating properties in terms of their electronic structure, aromaticity and their potential ability to bind metal ions. Carbaporphyrinoids realize the specific concept of macrocyclic ligand construction by fusing the structural frame of porphyrin and carbon donor(s) introduced by appropriately chosen moieties. The entrapment of metal ions in a coordination core of carbaporphyrinoids creates an efficient protection of the metal-carbon bond and allows to stabilize extremely rare oxidation/electronic states in organometallic environments. These macrocycles enforce the specific intramolecular reactivity and frequently exotic coordination architectures: **1-12**. The azulene moiety of azuliporphyrinoids provides the π -surface to bind the ruthenium cluster in a three-dimensional design of **11**. A contraction of *m*- or *p*-phenylene – embedded in *m*- or *p*-benzporphyrins **1**, **2** and **3** – to cyclopentadiene, mediated by metal cations produced complexes of 21-carbaporphyrins **4 - 7**. They reveal the unique inner core transformations including the reversible hydride or alkyl transfers. Noticeably, that the palladium(II) azulene-bridged A,D-dithiahexaphyrin undergoes the hydroxyl-triggered azulene contraction or isomerization to an oxynaphthalene unit of **12**, transforming the hexaphyrin framework into *meso*-linked carbaporphyrins. In due course one can expect that carbaporphyrinoids can prompt developments in organometallic chemistry building on “exotic” reactivity of built-in carbocyclic moieties.



Symposium : **ORGN3-3**

[Korea-Poland Joint Organic Chemistry Symposium] Recent Advances in Organic Chemistry in Cognate Areas of
Biology and Materials

Room 325A+B, FRI 15:30

Chair: Hee-Seung Lee (KAIST)

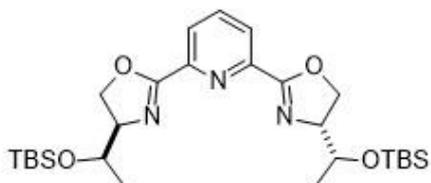
Zinc and Iron Catalysis in Asymmetric Synthesis

Jacek Mlynarski

Institute of Organic Chemistry, Polish Academy of Sciences, Poland

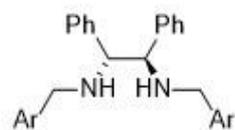
Asymmetric catalysis with the use of chiral metal complexes is still the most important method for the stereoselective formation of carbon-carbon and carbon-heteroatom bonds. After more than 40 years from the first use of transition metals for the catalytic asymmetric hydrogenation of alkenes and carbonyl compounds, the most efficient catalysts for these transformations are still compounds composed of rhodium, iridium, ruthenium or platinum. Recently, environmentally benign and less expensive catalysts have also been exhaustively explored leading to broad acceptance of earth-abundant metals such as zinc[1] and iron[2] in asymmetric synthesis. Previously our team showed that zinc[3] and iron[4] complexes can be efficient catalysts for many types of stereoselective additions to the carbonyl group including transformations in aqueous environment. Recently, we have also shown that the use of zinc complexes in the hydrosilylation reaction of prochiral ketones and imines can be much more efficient than application of platinum complexes.[5]References[1] Łowicki D., Baś S. Mlynarski J. Tetrahedron, 2015, 71, 1339.[2] Fürstner A. ACS Cent. Sci., 2016, 2, 778.[3] (a) Woyciechowska M., Forcher G., Buda S., Mlynarski J. Chem. Commun., 2012, 48, 11029; (b) Adamkiewicz A., Woyciechowska M., Mlynarski J. Eur. J. Org. Chem., 2016, 2897.[4] (a) Jankowska J., Paradowska J., Rakiel B., Mlynarski J. J. Org. Chem., 2007, 72, 2228; (b) Dudek A., Mlynarski J. J. Org. Chem., 2017, 82, 11218.[5] (a) Szewczyk M., Stanek F., Beżłada A., Mlynarski J. Adv. Synth. Catal., 2015, 357, 3727; (b) Beżłada A., Szewczyk M., Mlynarski J. J. Org. Chem., 2016, 81, 336; (c) Szewczyk M., Beżłada A., Mlynarski J. ChemCatChem, 2016, 8, 3575.

Zinc and Iron Catalysis in Asymmetric Synthesis
Jacek Mlynarski



Fe(OTf)₂ (10 mol%)
Mukaiyama in water

Fe(OTf)₂ (5 mol%)
asymmetric nitro-Mannich



Zn(OAc)₂ (0.05 mol%)
asymmetric hydrosilylation

Zn(OAc)₂ (5 mol%)
reductive aldol

Symposium : **ORGN3-4**

[Korea-Poland Joint Organic Chemistry Symposium] Recent Advances in Organic Chemistry in Cognate Areas of
Biology and Materials

Room 325A+B, FRI 15:55

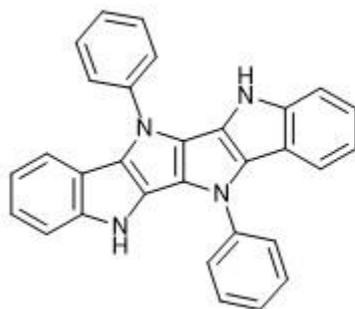
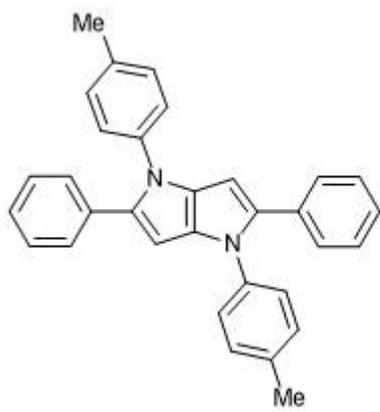
Chair: Hee-Seung Lee (KAIST)

Pyrrolo[3,2-b]pyrroles- electron-rich functional heterocycles

Daniel Gryko

Institute of Organic Chemistry, Polish Academy of Sciences, Poland

Recently we have discovered and optimized the first practical synthesis of non-fused pyrrolo[3,2-b]pyrroles via domino reaction of aldehydes, primary amines, and butane-2,3-dione [1]. Six bonds are formed in heretofore unknown tandem process, which gives rise to substituted pyrrolo[3,2-b]pyrroles – the ‘missing link’ on the map of aromatic heterocycles. Unparalleled simplicity and versatility of this one-pot reaction, non-chromatographic purification and superb optical properties (including strong violet, blue or green fluorescence both in solution as well as in the solid state), brought these molecules from virtual non-existence to the intensively investigated area functional π -systems. The parent 1,4-dihydro-pyrrolo[3,2-b]pyrroles served as building block to construct various π -expanded analogs including diindolo[2,3-b:2',3'-f]pyrrolo[3,2-b]pyrroles [2-4]. These compounds constitute the most electron-rich ladder-type heteroacenes known to date - HOMO was located at $\sim(-4.6)$ eV. Strongly fluorescent diindolo[2,3-b:2',3'-f]pyrrolo[3,2-b]pyrroles represent the longest ladder-type heteroacenes and the only existing compounds bearing the 1,4,5,8-tetrahydropyrrolo[3,2-b]pyrrolo[2',3':4,5]pyrrolo[2,3-d]pyrrole core.[1] M. Krzeszewski, B. Thorsted, J. Brewer, D. T. Gryko, *J. Org. Chem.*, 2014, 79, 3119.[2] B. Dereka, A. Rosspeintner, M. Krzeszewski, D. T. Gryko, E. Vauthey, *Angew. Chem. Int. Ed.* 2016, 55, 15624.[3] M. Krzeszewski, D. Gryko, D. T. Gryko, *Acc. Chem. Res.*, 2017, 50, 2334.[4] S. Mishra, M. Krzeszewski, C. A. Pignedoli, P. Ruffieux, R. Fasel, D. T. Gryko, *Nat. Commun.* 2018, 1714.



Symposium : **MEDI-1**

Current Trends in Drug Repositioning

Room 306B, THU 15:40

Chair: Minsoo Song (DGMIF)

Change positions and develop new drugs at half price!

Jin Keon Pai

1ST Biotherapeutics Inc., Korea

Despite the explosive development of biotechnology, the cost and duration of new drug development continues to increase, and the number of newly approved drugs by FDA/EMA is declining. To circumvent some of the most expensive drug discovery processes, companies pursue 'Drug Repositioning' strategy to increase their productivity (new drugs to market) by reducing the discovery and development timeline. 'Drug repositioning' identifies new therapeutic opportunities for existing drugs and compounds. This process seeks to discover new applications for an existing drug that were not previously referenced and not currently prescribed or investigated. This decreases the overall cost of bringing the drug to market because the safety and pharmacokinetic profiles of the repositioned candidates are already established.

Finding a good new drug development target is very difficult. Even though you identified new target, the biggest problem with 'drug repositioning' is it possesses a limited candidate substance for screen. There are only 4,000 compounds are available for screen including the FDA's approved substances. Using new methods such as DNA-encoded Libraries, you will be able to screen millions of candidate substances. Another problem is that if the drug value used in current usage of the candidate substance obtained through 'drug repositioning' is too low, it is causing a problem. Since we cannot exceed the current usage of low prices by the rules, the new usage will bring poor business. For example, you have identified the immune activator for drug repositioning. It is expected to respond very well to the "menstrual pain" that afflicts women. However, you must decide whether you must pursue further or not.

Glucagon-like peptide-1(GLP-1) receptor agonists are used for the treatment of type 2 diabetes mellitus with a low risk of hypoglycemia and the additional benefit of clinically relevant weight loss. Growing evidence suggests that agonists of the glucagon-like peptide 1 (GLP-1) receptor provide neuroprotection across a range of experimental models of Parkinson's disease (PD). Last year, a small proof-of-concept, open-label human trial of exenatide in the treatment moderate severity PD appeared to show persistent improvements in motor and cognitive function. The underlying mechanisms of action remain unclear, but

as evidence for the potential use of GLP-1 agonists in treating several neurodegenerative disease mounts, and with several clinical trials of GLP-1 analogues in PD and Alzheimer's disease (AD) currently underway. Here I would like to review this 'drug repositioning' of the neuroprotective effects of GLP-1 analogues for their potential therapeutic utility with relevance to PD and PD dementia (PDD).

Symposium : **MEDI-2**

Current Trends in Drug Repositioning

Room 306B, THU 16:05

Chair: Minsoo Song (DGMIF)

AI-driven Drug Repositioning and Beyond

Sang Ok Song

Standigm, Inc., Korea

With all the hype around AI, the adoption of AI within pharmaceutical industries has been increasing. How the AI-driven technologies are now explored at the entire stages of drug discovery and development is briefly reviewed focusing on major research partnerships between leading AI startups and big pharmaceutical companies. Standigm is one of leading companies in the “AI for drug discovery” space. The AI-based drug repositioning platform which is composed of three core AI modules, (1) Indication Prediction, (2) Prediction Interpretation, (3) Target Prioritization, generated tens of repurposed drug candidates for cancers, Parkinson’s disease, Non-alcoholic Fatty Liver disease and more, which have been experimentally validated. The most recent progress will be shared. Beyond repurposing of existing drugs, designing novel drugs is near at hand. How new molecules with better desired properties can be optimized from prototype molecules such as hits or leads will be summarized with example studies. In conclusion, technological and organizational challenges to overcome for successful AI application to drug discovery and development will be discussed. Standigm sees big progress towards overcoming them in coming years.

Symposium : **MEDI-3**

Current Trends in Drug Repositioning

Room 306B, THU 16:30

Chair: Minsoo Song (DGMIF)

CXCR4 hetromer as a drug target for precision cancer therapeutics

Dongseung Seen

R&D center, GPCR Therapeutics, Korea

CXC receptor 4 (CXCR4) is a member of the chemokine receptor family GPCR. CXCR4 responds to its ligand CXCL12/SDF-1, and has essential roles in the embryonic development of the hematopoietic, cardiovascular, and nervous systems. CXCR4 was discovered as a co-receptor for HIV, and has important roles in the homing of hematopoietic stem cells to the bone marrow, inflammation, immune surveillance of tissues, and tissue regeneration in adult. Overexpression of CXCR4 is regarded as a poor prognosis marker in many different types of human cancers including breast cancer, lung cancer, brain cancer, etc. CXCR4 plays pivotal roles in the proliferation, survival, and invasiveness of cancer cells. Various drugs targeting CXCR4 has been developed from AMD-3100, but development of CXCR4 antagonists as anti-cancer drugs is an ongoing challenge. To avoid potential side effects associated with conventional CXCR4 antagonists and to develop more efficient anti-cancer drugs targeting CXCR4, new paradigm for designing CXCR4 inhibitor is required. CXCR4 forms heteromers with different GPCRs. There exists a need for developing CXCR4 inhibitors for use as GPCR heteromer-targeting cancer therapeutics with higher efficacy and lower side effects. GPCR therapeutics Inc. was founded to develop CXCR4 heteromer inhibitors and has been validating using drug repositioning strategy. For the development of CXCR4 inhibitors, GPCR therapeutics and Samsung medical center have been collaborating in patient derived xenograft and antibody discovery. Up to now, GPCR therapeutics Inc. fund-raised about 12 million dollars from 7 Venture capitals in 2015 and 2016. Now, 25 persons work for GPCR therapeutics Inc.

Symposium : **MEDI-4**

Current Trends in Drug Repositioning

Room 306B, THU 17:10

Chair: Sang Min Lim (KIST)

Sharing Biologically-Relevant Compound Libraries and Bioassay Big-Data in Korea Chemical Bank

Hyeon Kyu Lee

Korea Chemical Bank, Korea Research Institute of Chemical Technology, Korea

Korea Chemical Bank (KCB) has been established 18 years ago for the purpose of supporting new drug discovery and chemical biology researches by sharing biologically-relevant compound resources in Korea. KCB also aims to promote collaborative researches between provider and user of compounds by sharing the information of hit compounds and screening results. Currently, KCB has about a half-million of diverse small mw organic compounds and single-component natural products collected from Korea research groups and strategically purchased from international vendors. Every year, KCB has supported more than 100 projects for new drug discovery and chemical biology researches in Korea providing several hundreds of thousands compounds. Till now, KCB has supported more than 800 HTS campaigns and the accumulated number of compounds provided is more than 6 million since year 2000. Through the 18 years operation of KCB, KCB has accumulated over 5 million of biological activity screening data for the provided compound libraries against more than 800 disease targets. With the 5M screening data information, KCB has started a new project for the implementation of medicinal information big-data platform to help new drug discovery and chemical biology researches in Korea by sharing the analyzed and curated medicinal information big-data with Korean researches. In this talk, the current status of KCB chemical libraries, managing system and the implementation of KRICT medicinal information big-data platform will be introduced.

Symposium : **MEDI-5**

Current Trends in Drug Repositioning

Room 306B, THU 17:35

Chair: Sang Min Lim (KIST)

Non-systemic drug discovery using aminoalkylbenzothiazepine derivative

Jaeho Yoo^{*}, Seungin Kim¹

Drug Discovery Center, drug discovery, Korea

¹New drug research center, CJ HealthCare, Korea

Non systemic drug stay and absorb only in small and large intestines. It can't absorb and means has merit during development because it doesn't need human ADME(DDI), human QT study and preclinical in vitro ADME screening. We found aminoalkylbenzothiazepine derivative can be compelling Non-systemic drug for treatment of constipation. It strongly inhibit IBAT transporter. Ileum bile acid transports (IBAT) are involved in reabsorbing bile acids into liver and Inhibition of IBAT increases amount of bile acid in large intestine. Increasing bile acid help colonic motility and fecal secretion. Laxatives are used but cause serious side effects (diarrhea, abdominal pain) and resistance. Recent prescription medications still suffer from low efficacy and slow onset time as well as nausea, diarrhea and CV concern. We believe non-systemic drug can solve this problem. To find candidate compound, we used ligand based drug discovery strategy. We designed using sulfone motif and long alky chain. Such as polar and bulky properties can help to be non-absorbable. Compound A is oral bioavailable and has high potency in IBAT in vitro assay. To check efficacy, the experimental rats administered with the compounds A excreted feces within a reduced time and also showed a significantly higher percentage in the number of rats regarding showed excretion of feces within 10 hours, compared to the control rats administered with vehicle. This suggests that the compound A can effectively prevent or treat constipation. Compound A exhibited potent and selective IBAT inhibition and effectively improved treatment constipation. These results warrant further investigation of compound A as a promising candidate for patient who needs treatment of constipation.

Symposium : **MAT1-1**

Frontier of Materials Chemistry: Application Fields

Room 322, THU 15:40

Chair: Younguk Kwon (Sungkyunkwan University)

Materials Design for Chemical Process Applications

Yong-Ki Park

Center for Convergent Chemical Process, Korea Research Institute of Chemical Technology, Korea

The petrochemical processes involved in manufacturing of chemical feedstock have been developed over the last 100 years and most of them have already been developed and optimized. However, the materials used in these processes still require much development. For example, new catalysts and separation materials with improved performance and new functionality are constantly needed to increase process efficiency of olefin production. Recently several processes using new materials have been reported. In particular, new materials such as MOF with new structures and chemical compositions have been developed and various attempts have been made to apply these materials to petrochemical reactions and separation processes. This talk will introduce new materials for chemical process applications under development in our research group and aims to attract the interest of many materials scientist.

Symposium : **MAT1-2**

Frontier of Materials Chemistry: Application Fields

Room 322, THU 16:20

Chair: Younguk Kwon (Sungkyunkwan University)

Electrocatalysts in Fuel Cells

Gu-Gon Park

Fuel Cell Laboratory, Korea Institute of Energy Research, Korea

Fuel cell technology has just started to be commercialized, and the market is rapidly growing mainly in cogeneration and automotive applications. In order to expand the market in earnest, R & D has been focused on the cost and the durability. The US Department of Energy estimates that the electrocatalyst portion of the entire fuel cell stack will account for about 48% in case of the annual production of 500,000 fuel cell vehicles. Two research directions are proposed to reduce the cost of electrocatalysts. One is to reduce the absolute amount of the precious metal, and the other is to increase the activity of the catalyst itself. To maximize the mass activity of the catalyst various approaches have been made through surface characterization and shape control (Dealloying, nano-segregation, nanoframe, octahedra, etc.). Considering mass production, now core shell type electrocatalyst is considered as a realistic alternative. In this presentation, we will share the prospect of current and future catalyst technologies based on a basic understanding of electrocatalysts.

Symposium : **MAT1-3**

Frontier of Materials Chemistry: Application Fields

Room 322, THU 17:00

Chair: Younguk Kwon (Sungkyunkwan University)

Ideal way of chemistry education for more effective industrial applications.

Jin-Kyu Lee

Corporate R&D, LG Chem, Korea

In a recent situation of the global competition, businesses are going to be more complex and having to respond faster than before because life cycles of products are getting shorter and competitors are not predictable anymore. Someone claims that the education at the universities is not suitable for the actual industrial situations and it has to be changed to more practical applications. However, in such a unpredictable situation, it is not even clear which direction is correct to go. When it comes down to it, the purpose of education is what it's all about! Several opinions based on my personal experiences will be discussed to find a better way making our students more trained to solve the new abnormal problems.

Symposium : **MAT2-1**

Frontier of Materials Chemistry: Photosciences

Room 322, FRI 14:30

Chair: Sungjin Park (Inha University)

Formation of Efficient Visible-Light Photocatalysts by Coupling of Semiconductors

Wan-In Lee

Department of Chemistry, Inha University, Korea

Design of advanced photocatalytic systems, effectively working under visible-light, is essential for practical application of photocatalysts in removing environmental pollutants. To achieve high efficiency, required properties for the photocatalysts will be profound solar light absorption in the visible-range, efficient charge-separation, suitable energy band locations for redox reactions, extended photostability, and others. Since a single semiconductor-based photocatalyst cannot satisfy all of these requirements, a potential strategy will be construction of coupled structures between two or more semiconductors. From this point of view, we explore various types of photocatalytic systems constructed by coupling of semiconductors and their working mechanisms. First of all, according to relative energy band positions between TiO₂ and visible-light sensitizers, different types of heterojunction were designed and their visible-light photocatalytic efficiencies were analyzed. In Type-A heterojunction, the conduction band (CB) level of sensitizer is positioned more negative side than that of TiO₂, whereas in Type-B system its valence band (VB) level is more positive than that of TiO₂. In evolving CO₂ from the gaseous 2-propanol (IP) under visible-light irradiation, the Type-B systems such as FeTiO₃/TiO₂, Ag₃PO₄/TiO₂, W₁₈O₄₉/TiO₂, Sb-doped SnO₂ (ATO)/TiO₂, FeWO₄/TiO₂ and others demonstrated noticeably higher photocatalytic efficiency than the Type-A such as CdS/TiO₂ and CdSe/TiO₂. Significantly higher visible-light photocatalytic activity of Type-B heterojunction structures could be explained by inter-semiconductor hole-transfer mechanism between the VB of sensitizer and that of TiO₂. In addition, p-n junction or Z-scheme based visible-light photocatalysts were designed and their photocatalytic mechanisms including charge-flow pathways are discussed intimately in this work.

Symposium : **MAT2-2**

Frontier of Materials Chemistry: Photosciences

Room 322, FRI 14:55

Chair: Sungjin Park (Inha University)

Next-Generation Light Emitters: Halide Perovskite Light-emitting Diodes

Tae-Woo Lee

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

Metal halide perovskites have emerged as promising next-generation light emitter due to their advantages such as high luminescence efficiency, high color purity, low material cost, solution processability, high charge-carrier mobility, and defect-tolerant electronic structure. Nevertheless, the low electroluminescence (EL) efficiency of perovskite light-emitting diodes (PeLEDs) at room temperature has been a big challenge which should be overcome. Here, we present high-efficiency PeLEDs using various strategies to overcome the EL efficiency limitations. First, we demonstrated a self-organized buffer hole injection layer to reduce the hole injection barrier and suppress the exciton quenching at the interface. Also, we showed that the formation of metallic lead clusters can cause strong exciton quenching and non-radiative recombination, which was prevented by finely increasing the molar proportion of methylammonium bromide (MABr) in MAPbBr₃ solution. Further, the EL efficiency could be dramatically enhanced by decreasing the size of MAPbBr₃ grains with improved uniformity and coverage of MAPbBr₃ layers. High-efficiency flexible MAPbBr₃ PeLEDs has been also demonstrated by using ideal anodes including graphene and ITO-free polymeric anode materials, which boosted the highest EQE up to 10.93% for pure green PeLEDs. We also developed mixed-cation systems with new substitute cations for MA using stable formamidinium (FA) and cesium (Cs), demonstrating first highly efficient and stable polycrystalline PeLEDs based on mixed cations. Furthermore, we developed efficient quasi-2D PeLEDs using Ruddlesden-Popper phase formed by incorporation of long alkyl cations and precise control over layered 2D structures.

Symposium : **MAT2-3**

Frontier of Materials Chemistry: Photosciences

Room 322, FRI 15:20

Chair: Sungjin Park (Inha University)

Light-Induced Modulation of Quantum Dot Conjugate Fluorescence

Sung Jee Kim

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

Photo-switching or modulation of quantum dots (QDs) can be promising for many fields that include display, memory, and super-resolution imaging. However, such modulations have been mostly relied on photo-modulations of conjugated molecules in QD vicinity which typically require high power of high energy photons at UV. We report a visible light-induced facile modulation route for QD-dye conjugates. QD crystal violets conjugates (QD-CVs) were prepared and the crystal violet (CV) molecules on QD quenched the fluorescence efficiently. The fluorescence of QD-CVs showed a single cycle of emission burst as they go through three stages of (i) initially quenched 'off' to (ii) photo-activated 'on' as the result of chemical change of CVs induced by photo-electrons from QD and (iii) back to photo-darkened 'off' by radical-associated reactions. Multi-color on-demand photo-patterning was demonstrated using QD-CV solid films. QD-CVs were introduced into cells, and excitation with visible light yielded photo-modulation from 'off' to 'on' and 'off' by nearly ten folds. Individual photoluminescence dynamics of QD-CVs was investigated using fluorescence correlation spectroscopy and single QD emission analysis, which revealed temporally-stochastic photo-activations and photo-darkenings. Exploiting the stochastic fluorescence burst of QD-CVs, simultaneous multi-color super-resolution localizations were demonstrated.

Symposium : **MAT2-4**

Frontier of Materials Chemistry: Photosciences

Room 322, FRI 15:45

Chair: Sungjin Park (Inha University)

Novel optical and magnetic property of self-doped colloidal nanocrystals

Kwang Seob Jeong

Department of Chemistry, Korea University, Korea

Size-dependent electronic transition is the prominent feature of quantum materials. Colloidal quantum dot is the most confined nanomaterial in dimension, showing the discrete electronic states even in the conduction band. The intraband transition, occurring between the quantized states of the conduction band of colloidal quantum dot, had been studied for the last two decades mostly by using ultrafast spectroscopy due to the fast hot-carrier relaxation. Recently, the steady-state intraband transition has been successfully observed from the self-doped nanocrystals. In this presentation, the novel optical, electronic and magnetic properties of the self-doped colloidal nanocrystals will be discussed, which had been a long-standing challenge in the colloidal nanocrystal field.

Symposium : **ELEC1-1**

Electrochemical Energy Conversion and Storage: Progress and New Challenges

Room 320, THU 15:40

Chair: Jun Ho Shim (Daegu University)

Elastic spongy graphene-functionalized silicon as excellent stability anode in Li ion battery

Chunfei Zhang, Jong-Sung Yu^{1,*}

Faculty of Maritime and Transportation, Ningbo University, China

¹Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Silicon can make alloy with lithium in the form of $\text{Li}_{22}\text{Si}_5$ to deliver a highest theoretical gravimetric capacity of $\sim 4200 \text{ mAh g}^{-1}$, and thus is considered to be one of the most promising anode materials for next generation Li ion battery. However, those advantages are seriously offset by a great challenge of large volume expansion during lithiation, which causes a serious damage to the electrode structure and thus gives rise to a fast decay of the specific capacity [1]. In this work, novel 3D spongy grapheme (SG)-functionalized silicon is for the first time demonstrated by chemical vapor deposition for a LIB anode, which can overcome the common silicon anode issues such as poor conductivity and volume expansion of Si as well as transfer of Li ion towards the Si. The elastic feature of graphene has excellent function to self-adaptively buffer the volume variation during charge-discharge process. In addition, different from traditional graphene or carbon shells (core-shell and yolk-shell), the spongy 3D graphene networks provide much improved unique functions with excellent long-cycle stability and rate capability. The Si@SG electrode exhibits excellent cycling performance with high reversible specific capacity [2]. A superior 95% capacity retention is achieved after 510 cycles. References[1] M. Zhou, X. Li, B. Wang, Y. Zhang, et al. Nano Lett. 15 (2015) 6222-6228. [2] C. Zhang, T.-H. Kang, J.-S. Yu, Nano Research, 11(2018) 233-245.

Symposium : ELEC1-2

Electrochemical Energy Conversion and Storage: Progress and New Challenges

Room 320, THU 16:05

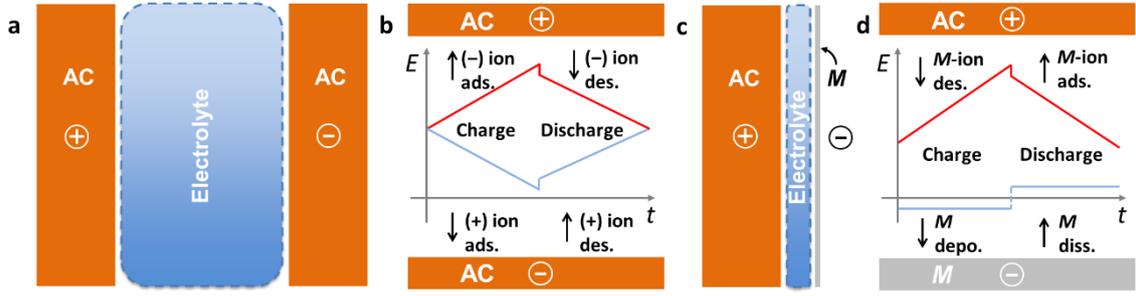
Chair: Jun Ho Shim (Daegu University)

'Rocking-Chair'-type Metal Hybrid Supercapacitors

Hyun Deog Yoo

Department of Chemistry, Pusan National University, Korea

Supercapacitors can provide high rate capability and long-term cycleability, thanks to their simple mechanism based on the adsorption and desorption of ions on the surface of electrodes. Based on the high power characteristics, supercapacitors can augment the batteries or fuel cells for electric vehicles or heavy equipment. So far, most of supercapacitors have symmetric configuration with activated carbon electrodes as the positive and negative electrodes (Fig. 1a). And they follow a Daniell-type mechanism, where the electrolyte is depleted of and replenished with ions upon charging and discharging, respectively (Fig. 1b). In this mechanism, electrolyte serves as an ionic reservoir, from which cations and anions are separated to negative and positive electrodes, respectively. This leads to a limitation in energy density and an increase in the internal resistance as the starvation of the concentration of salts in the electrolyte decreases during operation. Herein, we introduce a hybrid supercapacitor that follows a 'rocking-chair' mechanism. This hybrid supercapacitor is composed of metal anodes and activated carbon as the negative and positive electrodes, respectively (Fig. 1c). Metal (M, e.g. Mg or Zn) ions are replenished at the negative electrode while they are adsorbed into the pores of the positive electrode upon the discharging of the cell (Fig. 1d). As a result, only a minimum amount of electrolyte is needed to operate the cell. The use of metal electrodes can increase the energy density of the cell significantly by virtue of the large volumetric capacity. Therefore, 'rocking-chair'-type metal hybrid supercapacitors can double the energy density of a supercapacitor. Detailed studies on the 'rocking-chair'-type mechanism will be presented.



Symposium : **ELEC1-3**

Electrochemical Energy Conversion and Storage: Progress and New Challenges

Room 320, THU 16:30

Chair: Jun Ho Shim (Daegu University)

Corrosion engineering toward high-performance electrodes for oxygen evolution and water splitting

Byungkwon Lim

Sungkyunkwan University, Korea

Corrosion is generally considered to be an undesirable process that leads to damage and failure of a material, typically a metal or alloy, but understanding and control of surface processes involved in corrosion may enable its utilization in a more productive way. We show that simply by corroding Ni foam in an aqueous solution, it is possible to produce high-performance oxygen evolution electrodes. When Ni foam was corroded in water or an aqueous solution containing NaCl, a dense array of Ni(OH)₂ nanosheets was produced on the surface of the foam. When corroded in the presence of RuCl₃, the nanostructured surface composed of Ni(OH)₂ nanosheets decorated with ultrasmall RuO₂ nanoparticles was obtained. At an applied voltage of 1.7 V, the combination of these two nanostructured surfaces yielded a water-splitting current density more than three times that obtained on the commercial Pt wire electrodes. Furthermore, we also fabricated a high-performance OER electrode consisting of a dense array of ternary NiFeCo layered double hydroxide (LDH) nanosheets by corroding a Ni foam in an aqueous solution containing Fe³⁺ and Co²⁺ cations. This electrode exhibited a small overpotential of 170 mV at current density of 10 mA cm⁻² in 1 M KOH. This OER electrode was coupled with a CoP-based hydrogen evolution reaction electrocatalyst to construct an alkaline electrolyzer, which achieved the current density of 10 mA/cm² only at an applied voltage of 1.49 V in 1 M KOH. It is anticipated that our approach could also be extended to fabricate ternary or higher LDH electrodes with desired compositions for OER and other catalytic applications.

Symposium : **ELEC1-4**

Electrochemical Energy Conversion and Storage: Progress and New Challenges

Room 320, THU 16:55

Chair: Jun Ho Shim (Daegu University)

Research and Application of Reinforced Composite Polymer Electrolyte Membrane in Fuel Cell for Transportation Applications

Jin Young Kim

Fuel Cell Research Center, Korea Institute of Science and Technology, Korea

A polytetrafluoroethylene (PTFE)-reinforced perfluorosulfonic acid (PFSA) composite material is a cost effective alternative to the pure polymer electrolyte, which is often applied as polymer electrolyte membrane in fuel cell for transportation applications simply by infiltrating PFSA ionomer solution into porous PTFE matrix. For the membrane production, the reduction in cost and electrolyte thickness is an attractive factor, but it is still a challenge to produce the composite membranes as efficient as commercial membranes. Recent research and application activities with the reinforced composite membrane for the fuel cell applications include infiltration of the PFSA ionomer into the PTFE support, improving proton conductivity, reducing gas permeability, and addition of radical scavengers. In this talk, our recent results from these activities will be presented.

Symposium : **ELEC1-5**

Electrochemical Energy Conversion and Storage: Progress and New Challenges

Room 320, THU 17:20

Chair: Jun Ho Shim (Daegu University)

Interconnected Silicon Nanoparticles via Carbon Network Derived from Cellulose Nanofibers for Lithium Ion Battery Anodes

Yuanzhe Piao

Graduate School of Convergence Science and Technol, Seoul National University, Korea

The application of nanocellulose-based scaffolds as precursors for electrode materials can result in cost-effective materials. In this work, pyrolysis of three-dimensional wood-based lignocellulosic materials was studied for the preparation of lithium ion battery electrodes with high surface area and adjustable porosity to obtain conductive open networks that show a high electronic conductivity. Preliminary experiments using pyrolysed nanocellulose aerogels have shown that, by increasing the micropore volume and tailoring them to specific electrolytes, higher specific capacitances could be obtained. Ultrathin cellulose nanofibers entangle each silicon nanoparticle and become extensively interconnected carbon network after pyrolysis. This wide range interconnection provides an efficient electron path by decreasing the likelihood that electrons experience contact resistivity and also suppresses the volume expansion of silicon during lithiation. In addition, ultrathin cellulose nanofibers are carboxylated and therefore adhesive to silicon nanoparticles through hydrogen bonding. This property makes ultrathin cellulose the perfect carbon source when making silicon composites. As a consequence, it exhibits 808 mAh g⁻¹ of the reversible capacity after 500 cycles at high current density of 2 A g⁻¹ with a coulombic efficiency of 99.8 %. Even at high current density of 8 A g⁻¹, it shows a high reversible discharge capacity of 464 mAh g⁻¹. Moreover, extensively interconnected carbon network prevents the formation of a brittle electrode with a water-based binder. Therefore, this remarkable material has a huge potential for lithium-ion battery applications.

Award Lecture in Division : **ELEC2-3**

Recent Trends in Physical and Analytical Electrochemistry

Room 320, FRI 10:20

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

What Can Electrochemical Interface Tell Electrochemists? The Case Studies of Advanced Electrodes for Energy Storage Devices

Jin Ho Bang

Department of Bionano Technology and Department of Chemical and Molecular Engineering, Hanyang University, Korea

Understanding electrochemical interface is crucial in establishing a new design principle of advanced electrodes for energy applications. However, the ability to control the interface is still limited, and elucidating the resulting performance trend remain a big challenge to electrochemists. In this symposium, our efforts to gain insight into various interfacial phenomena are presented, in particular focusing on a new comprehensive understanding of carbon/electrolyte interfaces that are frequently encountered in energy storage devices.

Symposium : ELEC2-1

Recent Trends in Physical and Analytical Electrochemistry

Room 320, FRI 09:20

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Large-scale reverse electrodialysis operated by water electrolysis in neutral-pH water

Jihyung Han, Namjo Jeong¹, Chan-Soo Kim^{1,*}

Marine Energy Convergence & Integration Laboratory, Korea Institute of Energy Research, Korea

¹*Korea Institute of Energy Research, Korea*

Reverse electrodialysis (RED) produces electric power from mixing sea water with river water, with the stack voltage increasing proportionally up to several dozens of volts as the number of ion exchange membranes increases. Under these conditions, water electrolysis is a realistic redox reaction to convert ion flow into electron flow, because voltage loss by electrode resistance is much smaller than the total stack voltage. In this study, RED system includes a high membrane voltage from more than 50 cells, neutral-pH water as the electrolyte, and an artificial NaCl solution as the feed water, which is more universal, economical, and eco-friendly than that reported previously. We demonstrate that even though there is no specific method to reduce the overpotential for water electrolysis, large stack voltage with more than 50 cells can utilize the water oxidation/reduction in neutral-pH media as the electrode reaction in RED systems. All hydrogen gas produced at maximum power of RED is collected using a batch-type electrode chamber without electrolyte circulation and its production rate is $1.1 \times 10^{-4} \text{ mol cm}^{-2} \text{ h}^{-1}$, which is larger than previously reported values for RED-driven hydrogen production. Therefore, when a pilot-scaled RED consisting of hundreds of cell pairs is operated, water electrolysis in neutral-pH electrolyte can be an effective redox reaction to produce not only electric power but also hydrogen energy. Overall, we expect this RED system to stimulate the sustainable energy community and the eco-friendly hydrogen economy, providing a new paradigm for future research initiatives. This research was supported by the Technology Development Program to Solve Climate Changes of the National Research Foundation (NRF) funded by the Ministry of Science, ICT & Future Planning (2017M1A2A2047366).

Symposium : ELEC2-2

Recent Trends in Physical and Analytical Electrochemistry

Room 320, FRI 09:50

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

An Alternative Choice of the Glass Membrane pH Electrode: Nano-IrO₂ Polymeric Composite pH Electrode

Jongman Park

Department of Chemistry, Konkuk University, Korea

The main stream tool of practical pH sensing has not been changed from the glass membrane pH electrodes for more than half century. Excellency of the hydrogen ion selectivity of the glass membrane pH electrodes without alternative choices has being held the users in all the area of sciences and industries, although it is fragile, not easy to treat, and even expensive. Metal oxide-based hydrogen ion film electrodes have been studied extensively for long time because of their high sensitivity to the hydrogen ion. However they are not satisfactory for practical uses due to the lack of stability, reproducibility, and severe drifts caused by the microscopic porosity, cracks or non-uniformity of the films formed during sputtering, thermal decomposition or electrochemical deposition. Great efforts have been made to overcome such problems in the metal oxide-based pH electrodes utilizing the composite electrode technique. Various pH sensing materials, conductors, and matrices have been examined, and then finalized to nano-iridium oxide polymeric composite pH electrode as an alternative choice of the glass membrane pH electrode. In this symposium the ways of research in composite pH sensing electrode and efforts for real world pH sensing will be presented.

Symposium : **EDU1-1**

Current Issues and Research in Chemistry Education

Room 315, THU 15:40

Chair: Aeran Choi (Ewha Womans University)

Past and Prospects of the Chemistry Test in the SU-NEUNG; How it has been changed and how it should go

Chinkap Chung

Department of Chemistry, Keimyung University, Korea

Recently, the 2022 university entrance system including the SU-NEUNG (Korean college scholastic ability tests) according to the 2015 revised curriculum becomes social hot issues. Issues included are the role of the SU-NEUNG in college entrance, whether absolute evaluation or relative evaluation, and inclusion of science II subjects. Since the SU-NEUNG is the major element in the admission selection process for universities in Korea, not only parents, but also science and technology, industry, etc. are greatly interested in this test. The proportions and the details of questions of chemistry in the SUNEUNG will give a great impact on the high school chemistry classes and eventually college chemistry classes. In this presentation, the details of how the chemistry test in the SU-NEUNG has been changed during the past 25 years of SU-NEUNG history will be discussed as well as the prospects of changes of the SU-NEUNG.

Symposium : **EDU1-2**

Current Issues and Research in Chemistry Education

Room 315, THU 16:10

Chair: Aeran Choi (Ewha Womans University)

ANALYZING TREND OF CHEMISTRY ITEMS IN THE JAPANESE COLLEGE ENTRANCE EXAMS

Young Tae Kong

General Science Education, Chinju National University of Education, Korea

In this study, we analyzed the trends of chemistry items in the Japanese college entrance exams (unification test and university test) in order to obtain basic data for improvement of chemistry items in Korea's entrance examination. The research subjects used in this study include the unification test that corresponds to the Korean SAT in the last five years and the items that each university in Japan conducts itself. Among them, we have extracted the items corresponding to Chemistry I and Chemistry II in our country. The analysis of questions was divided into behavior and content domain, and content domain was subdivided into knowledge, inquiry, and attitude. In addition, comparative study of the entrance examination items of Japan and Korea was conducted.[1] H.K. Kim (2010). Item analysis of Japanese NCTUA for the quality improvement of chemistry items of CSAT. Journal of the Korean Chemical Society, 54(6), 818-828. Acknowledgments: This work was supported by National Research Foundation of Korea Grant funded by the Korean Government (NRF-2016R1D1A1B02008712).

Symposium : **EDU1-3**

Current Issues and Research in Chemistry Education

Room 315, THU 16:40

Chair: Aeran Choi (Ewha Womans University)

Why did the number of students selecting chemistry I gradually decrease?: Focusing on teacher's perspective

Sungki Kim

Gwangju Science Academy for the Gifted, Korea

The proportion of students selecting chemistry I has been gradually decreasing from the 2014 College Scholastic Ability Test(CSAT) to which the 2009 revised curriculum applies. Even students entering a chemistry-related college tend to do not choose chemistry. The purpose of this study is to analyze these problem from the teachers' viewpoint and to draw up a solution plan. The subjects of this study were 24 chemistry teachers who had the experience teaching students preparing CSAT applying the 2009 revised curriculum. First, they asked to respond in a narrative form to the questionnaire consisting of fulfillment of the curriculum, the difficulty of the questions, and guidance on the killer items etc. After that, the reasons for the whole response with 7 focus teachers are analyzed. About the reasons for the decrease in the number of students for chemistry I, the chemistry teachers think that ①the item that evaluates mathematical ability rather than the chemical ability, ②the killer item which actually kills chemistry selection, ③the ambiguity about the fulfillment of the curriculum, ④big gap between the textbook and CSAT items. The CSAT should be an assessment of the ability to be able to study a university's course especially with regard to the major. In this respect, current chemistry I items in CSAT should be revised to focus more on the ability assessment of chemistry.

Symposium : **EDU2-1**

Chemistry Education for the Science Gifted Students

Room 315, FRI 14:30

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Korea Science Academy Organic chemistry class for the scientific gifted students

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

Organic chemistry is one of the chemistry enrichment courses of the gifted school. At the Korea Science Academy, there are chemistry enrichment courses such as fundamentals of organic chemistry, introduction to nanochemistry, fundamentals of analytical chemistry, chemistry and energy, and introduction to spectroscopy. Students with interests and talents in the chemistry field choose to study these enrichment courses. These chemistry curriculum provides knowledge at university level to students interested in chemistry. And also it provides the necessary deepening knowledge in the second year R&E research activities and third year graduation research activities. Organic chemistry classes provide team discussion to help students understand the reactivity of organic compounds by functional groups while solving the problems given to the groups together. Students draw on organic reaction mechanisms to understand the structure and reactivity of organic compounds. Students do an organic synthesis team project that they are interested in and conduct organic synthesis project activities as a semester project. In this presentation, I will share the process of studying organic chemistry through group activities.

Symposium : **EDU2-2**

Chemistry Education for the Science Gifted Students

Room 315, FRI 14:40

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

A Study on the Viewpoint of Gifted School Students' Science Philosophy with Essay Evaluation

Se hee Park^{*}, Yon Li Jeong

chemistry, Gyeonggi Science High School for the Gifted, Korea

In this research, we examine, through discussion, the process of generating scientific theories from the viewpoint of modern science philosophy, and explore various scientific philosophies gifted students have. After presenting the structure of Thomas Samuel Kuhn's scientific revolution, a modern science philosophy, and the reference material of the research program of Lakatos Imre, the students interpret the process of changing the definition of the Acid-base group based on Kuhn's philosophy and Lakatos's research. Hereafter, the process of the evolution of the scientific theory is explained and the process of the atomic model change is analyzed in terms of Kuhn and Lakatos. Through this process, we observed how students' views of existing scientific philosophies change. As a result, the recognition of the six topic scientific research methods have developed in the hypothesis-deductional way, which is a more evolved method, In regard to evidence collection and analysis, observation of experiments, theories, laws, model, the students' perspective have shifted from the observational inductive perspective to hypothetical-deductive perspective.

Symposium : **EDU2-3**

Chemistry Education for the Science Gifted Students

Room 315, FRI 14:50

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Introduction of Process-Based Performance Evaluation on Chemistry Course in Gifted school

Youngkyong Kim

Daegu Science High School, Korea

In the 2015 revised curriculum, process-based assessment is emphasized. and In the inquiry-oriented science class, the evaluation should be process-based. Currently, process-based evaluation is actively conducted in middle schools and general high schools. but, gifted School does not emphasize the importance of a process-based evaluation. The Open Ended Project, which is currently undergoing process-oriented evaluation of the general chemistry experiment 1 course currently being held at Daegu Science High School, is introduced. and I want to be able to use it in chemistry-related subjects. The Open Ended Project presents students with seven project topics presented as group activities, selects one of them, and conducts the entire process from preparation for experiment, design, interpretation of results, and conclusion to the students themselves. The purpose of this project is to improve students' problem solving and personal skills. There are no set answers, and they are evaluated according to how to plan, conduct experiments, analyze and interpret results and report quality. Through this process, the process - based evaluation in science gifted high school will be activated.

Symposium : **EDU2-4**

Chemistry Education for the Science Gifted Students

Room 315, FRI 15:00

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Developing Process-Focused Assessment in Science High School Chemistry Class

Daeseong Jin

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

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

Symposium : EDU2-5

Chemistry Education for the Science Gifted Students

Room 315, FRI 15:10

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Evaluation of the experimental practice in the lecture subject

Jurae Kim

Department of Chemistry, Seoul Science High School, Korea

The curriculum of our school consists of a separate class of theoretical and experimental classes. As a result, it is difficult to experience experiments related to class contents and it is necessary to carry out experiments related to class contents separately from experiment classes. However, experiments that do not overlap with experimental classes should be conducted. Under the theme of chemical cell and electrolysis, students conducted an open experiment to construct a battery by selecting from the given conditions, giving students an opportunity to learn the practical skills required for the experiment and compare the experimental results according to various conditions. Lesson Results The students showed interesting reactions such as constructing and comparing chemical cells under various conditions, not the conditions presented in the textbooks, or constructing chemical cells that exceed the limitations of the given conditions by changing the substances with additional chemical reactions.

5. 과정, 결과 및 분석

[실험과정]

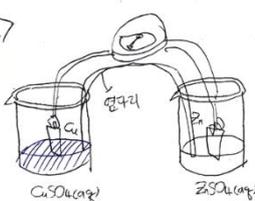
<실험I>
(불타전지)



① 전극을 시판으로 갖는다
 ② 포화 NaCl 용액을 준비하였다
 ③ 전압계와 전류에 따라 두가지 전극들을 H_2O 또는 H_2O_2 가 첨가했다.
 ③ 각각의 측정된 전압을 기록하였다

아연전극, 구리전극, 마그네슘전극, 납전극, 알루미늄전극

<실험II>
(다발전지)



① CuSO_4 와 ZnSO_4 용액은 같은 농도 (몰농도)로 준비
 ② 전압계를 사용하여 두서너개의 전압 측정
 ③ 두 용액의 농도를 바꾸어 여러 전압 측정

* 6가지 조합의 기전력

사용한 용액	전극	전압 (V)	전류 (mA)
(+) $\text{CuSO}_4(aq)$ 0.1M	Cu	1.054	0.94
(-) $\text{ZnSO}_4(aq)$ 0.1M	Zn		
(+) $\text{CuSO}_4(aq)$ 0.1M	Cu	1.755	1.93
(-) $\text{MgCl}_2(aq)$ 0.1M	Mg		
(+) $\text{CuSO}_4(aq)$ 0.1M	Zn	0.608	0.90
(-) $\text{MgCl}_2(aq)$ 0.1M	Mg		
(+) H_2O_2	C	1.090	0.93
(-) $\text{ZnSO}_4(aq)$ 0.1M	Zn		
(+) H_2O_2	C	1.420	1.09
(-) $\text{CuSO}_4(aq)$ 0.1M	Mg		
(+) $\text{CuSO}_4(aq)$ 0.1M	Cu	0.220	0.11
(-) H_2O	C		

Symposium : **EDU2-6**

Chemistry Education for the Science Gifted Students

Room 315, FRI 15:20

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Practice of Artistic Biochemistry Class

Sumi Seong

Sejong Academy of Science and Arts, Departments of Chemistry, Korea

The Artistic Biochemistry is a kind of creative fusion subjects based on 100% performance evaluation. This subjects helps students understand the core concepts of Life science and Chemistry by dealing with phenomena and by challenging the problems related with Life science and Chemistry. It aims to make students interested in Life science, Chemistry and why they study these subjects. To do this, we organize classes by experimenting with life and chemical phenomena, discussing the Nobel Prize in Physiology and Chemistry, and explaining the phenomena by the core concepts of Life science and Chemistry. One of them is a biomimetic phenomena lesson, which allows students to experiment with the Lotus effect. It also makes the students propose the invention items that can be used innovatively in everyday life by using the Lotus effect and to write the booth proposal that introduces the Lotus effect to the public. And this lesson makes the students take photographs of the beautiful phenomenon observed in the Lotus effect experiment and cheers them up to exhibit at a science photo contest. We intended the students to feel the beauty in the science phenomenon. We would like to introduce the practical examples of the class including this.



Symposium : EDU2-7

Chemistry Education for the Science Gifted Students

Room 315, FRI 15:30

Chair: Daeseong Jin (Daejeon Science High School for the Gifted)

Process-based Evaluation in Gwangju Science Academy for the Gifted

Donggeon Lee

Gwangju Science Academy for the Gifted, Korea

This study analyzed the actual situation of the process-based evaluation through Gwangju Academy's case of the chemistry class time. Through this, we aim to derive an authentic evaluation method for gifted education. This study was conducted based on the performance evaluation conducted in chemistry class at Gwangju science gifted school in the first semester of 2018. Then, the evaluation was carried out based on the teacher's point of view derived from student's output, self-report, and observation in class. As a result of the research, it was found that the participation of the students in the class was improved through the process-based evaluation and it was effective in fostering the fusion literacy. However, problem of the education system of the entrance examination system, the problem of the establishment of the objective evaluation standard, and the securing of the fairness make relatively difficult to operate according to the original purpose of the process-based evaluation. Based on the results of this study, we will share practical examples of the process-based evaluation conducted by gifted schools across the country and discuss the operation method.

Symposium : **ENVR-1**

R&D beyond Carbon Society II

Room 306A, THU 15:40

Chair: Jaeyoung Lee (GIST)

Computational Design of Efficient Catalyst for NH₃ Decomposition and Synthesis

Hyung Chul Ham

Fuel Cell Research Center, Korea Institute of Science and Technology (KIST), Korea

Today, the human society strongly relies on the fossil fuels for the energy sources. However, the environmental crisis (such as the global warming, and pollutant discharge) caused by the use of fossil fuels and the depletion of fossil fuels drives the human beings to develop the new alternatives to fossil fuels. The hydrogen energy has been considered to be the promising option for simultaneously solving such energy and environmental issues. One of bottlenecks for attaining the hydrogen-powered society is to find the efficient hydrogen carrier. Among various hydrogen carriers, ammonia has received much attention in recent years due to the high gravimetric (17.8wt% H₂) and volumetric (121 kg H₂ m⁻³ in the liquid form) hydrogen density. For the effective application of ammonia to the hydrogen carrier, the highly active catalyst for ammonia decomposition and synthesis should be developed. However, a detailed understanding of how to control the activity of catalysts is still lacking, despite its importance in designing and developing new effective ammonia decomposition and synthesis catalysts. This is in large part due to the difficulty of direct characterization. Alternatively, quantum mechanics-based computational approaches have emerged as a powerful and flexible means to unravel the complex catalysis in nanocatalysts. In this talk, I will present the recent research activity on the design of highly efficient ammonia-related catalysts using first-principles density functional theory(DFT) and machine learning approach.

Symposium : **ENVR-2**

R&D beyond Carbon Society II

Room 306A, THU 16:15

Chair: Jaeyoung Lee (GIST)

Advanced separators for safe Li-ion batteries

Jung-Je Woo

Gwangju Bio/Energy R&D Center, Korea Institute of Energy Research, Korea

Lithium ion batteries have been using as representative energy storage systems for various applications. To improve battery safety, a battery separator should prevent internal short circuit under abnormal condition. Most of the current separators are based on polyolefins, such as polyethylene and polypropylene, which lose mechanical integrity over 150°C. In this study, we developed a thermally stable separator based on a poly (phenylene oxide)/SiO₂ composite by a dry phase inversion method. The separator endures up to 250°C without obvious thermal deformation. A NMC/graphite cell using the composite separator showed excellent cycling performance, especially at high C-rates. This separator layer was directly coated on an anode to form a separator/electrode assembly (SEA), which offers enhanced interfacial properties, high mechanical strength, and thermal stability. Another way to improve safety of batteries is to reduce the flammability of the liquid electrolyte. A new flame retarding separator (FRS) based on brominated poly (phenylene oxide)(BPPO) remarkably reduced the flammability of the liquid electrolyte without decrease in electrochemical performances such as ionic conductivity and cycle life of a lithium-ion battery.

Symposium : **ENVR-3**

R&D beyond Carbon Society II

Room 306A, THU 17:00

Chair: Jaeyoung Lee (GIST)

Electrosynthesis for Energy and Environment

Youngkook Kwon

Korea Research Institute of Chemical Technology, Korea

The efficient 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, as it would allow for the direct low-temperature conversion of photo-generated electrical current to stored chemical energy, in a manner very similar to the way nature stores solar energy. The high activity and selectivity towards electrocatalytic conversion of CO₂ can be achieved with careful selection of catalyst and electrolyte. In addition, ammonia (NH₃) synthesis, mainly for fertilizers, from N₂ has been performed via the Haber-Bosch process at high temperature and pressure, consuming large amount of H₂ from fossil resources and more than 1% of the total fossil energy consumption on Earth. Instead, the development of an efficient electrochemical process to generate carbon-neutral NH₃ under ambient conditions using renewable energy sources becomes essential. In this talk, recent attempts for efficient electrosynthesis of value-added chemicals will be introduced.

Symposium : **ENVR-4**

R&D beyond Carbon Society II

Room 306A, THU 17:30

Chair: Jaeyoung Lee (GIST)

Advanced nanostructured TiO₂ and its energy applications

Kiyoung Lee

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

There has been a considerable interest in one-dimensional nanostructures owing to their remarkable characteristics in particular these electronic properties which have been considered to significantly improve the electron transport time and reduce the recombination rate. The range of research area of one-dimensional nanostructures covers meanwhile a wide range of transition metal oxides. Among them, TiO₂ is the most widely studied material because of its promising applications in solar-cells, photoelectrochemical hydrogen production, and CO₂ reduction etc.. Because, highly aligned TiO₂ nanostructures have been suitable semiconductive properties with ~ 3 eV and optimum band-edges to water, fast electron path way, and chemical stability. In order to form such one-dimensional TiO₂ nanostructures, a most straight forward approach is considered to direct electrochemical anodic reactions (named anodization) on Ti metal substrate in a dilute fluoride containing electrolyte. This approach is very simple and easy to control dimensions (diameter and length) and structure. In this presentation, we will show the growing mechanism of anodic TiO₂ nanostructures and further modification of the anodic structure for energy application such as solar cells, photocatalytic hydrogen evolution.

122nd General Meeting of the Korean Chemical Society
October 17(Wed)~19(Fri), 2018, EXCO, Daegu, Korea

Symposium : **KCS1-1**

[IBS Symposium] Recent Advances in Carbon Materials

Room 321, WED 15:00

Chair: Rodney S. Ruoff (IBS CMCM)

Aromatic Architectures based on Corannulene

Jay S. Siegel

Health Science Platform, Tianjin University, United States

An expose of the design, synthesis and physical studies of aromatic architectures based on corannulene.

Symposium : **KCS1-2**

[IBS Symposium] Recent Advances in Carbon Materials

Room 321, WED 15:45

Chair: Christopher Bielawski (IBS CMCM)

Chemically induced transformation of CVD-grown bilayer graphene into single layer diamond

Pavel Bakharev

CMCM, IBS Center for Multidimensional Carbon Materials, Korea

In this work, we report on the first experimental observation of the fluorine chemisorption induced sp² to sp³ phase transition of large-area bilayer graphene to diamond-like film under moderate conditions (near-room temperature and at a low pressure (less than one atmosphere and the structure is stable at 1 atm)). The synthesis of a novel ultra-thin diamond-like material, namely fluorinated diamond monolayer ('F-diamane'), has been achieved in two ways. The first is the fluorination of bilayer graphene on single crystal metal (CuNi(111) alloy) foil, on which the bilayer graphene was grown by chemical vapor deposition (CVD). The other is fluorination of the same type of CVD bilayer graphene film transferred onto TEM (transmission electron microscopy) gold grids to obtain F-diamane film "suspended" on a chemically inert support. Our spectroscopic, transmission electron microscopy, and density functional studies unequivocally show that the fluorine chemisorption on CVD-grown bilayer graphene under certain conditions results in formation of F-diamane.

Symposium : **KCS1-3**

[IBS Symposium] Recent Advances in Carbon Materials

Room 321, WED 16:15

Chair: Christopher Bielawski (IBS CMCM)

Chemical environment dependent growth of transition metal dichalcogenides: a computational study

Wen Zhao, Feng Ding*

Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS), Korea

Transition metal dichalcogenides (TMDCs) are a large family of 2D materials with a wide spectrum of properties. I first introduce a collaborative work about the vapor-liquid-solid (VLS) growth of MoS₂ ribbons by salt-assisted CVD. Compared to conventional vapor-solid growth, the formation of molten Na-Mo-O-S droplets allows the rapid deposition of precursors at the interface between the droplet and the TMDC and, therefore, drastically increases the growth rate by orders of magnitude. Then I will talk about our theoretical work on the nucleation of MoS₂. A large number of isomers of Mo_xS_y clusters ($x = 1, \dots, 10$, and $y = x, \dots, 3x$ or more) have been evaluated. We have found that (i) a few highly stable and also small Mo_xS_y ($x = 1, 2, 3$) clusters are predicted to be the precursors of MoS₂ growth, and (ii) a series of phase transitions from 3D structures to planar T-phase, and then to planar H-phase TMDC configurations are predicted as the possible 'evolutionary path' in TMDC growth.

Symposium : **KCS1-4**

[IBS Symposium] Recent Advances in Carbon Materials

Room 321, WED 16:45

Chair: Christopher Bielawski (IBS CMCM)

Oxidized Carbons: New Catalysts for Synthetic Reactions

Hyosic Jung, Christopher Bielawski^{1,*}

Chemistry, Ulsan National Institute of Science and Technology, Korea

¹*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

Catalysts are often utilized to facilitate chemical reactions. Although metal based-catalysts are commonplace and have been well studied in the context of a wide variety of transformations, a number of drawbacks are evident, including high costs, toxicity concerns, and recyclability limitations. It has been hypothesized that oxidized carbons may be used as alternatives to metal-based catalysts. In this presentation, I will describe the preparation of various types of oxidized carbons and demonstrate how they may be used to promote a broad range of small molecule and macromolecular transformations. The integration oxidized carbons with contemporary techniques of synthetic chemistry will also be discussed.

Symposium : **KCS1-5**

[IBS Symposium] Recent Advances in Carbon Materials

Room 321, WED 17:15

Chair: Christopher Bielawski (IBS CMCM)

Metal doped graphene or carbon nanotubes for electrocatalysts and graphene nanoribbons for 2D molecular electronics spectroscopy

Kwang Soo Kim

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

I will discuss metal doped or hybrid carbon materials for electrocatalysts and graphene nanoribbons (GNRs) for electronics/spintronics, and 2D molecular electronics spectroscopy (2D-MES). To design a catalyst showing superior activity for a specific electrochemical reaction, a specific single metal atom can be embedded into doped graphene. As an example, we grew graphitic tubes (GTs) using melamine in the presence of Fe/Co/Cu through heating in an N₂ gas atmosphere. Then, FeCo₃ nanoparticles are encapsulated inside GTs. Further, on GT surface an ultralow amount of Pt (only ~1 μg) was electrochemically deposited. Then, Pt single atoms were embedded in GT surface, while some Pt clusters were additionally formed on GT surface. The synergistic effect between the Pt clusters and single Pt atoms significantly enhanced the catalytic activity for hydrogen evolution. With a 1/80th Pt loading of a commercial 20% Pt/C catalyst, in 0.5 M H₂SO₄, the catalyst achieved 10 mA cm⁻² at an overpotential of 18 mV, and showed a turnover frequency of 7.22 s⁻¹ (96 times higher than that of the Pt/C catalyst) and long-term durability [Nat. Energy 2018]. Such remarkable efficiency originates from small free energy of H adsorption of single Pt atoms coordinated by C₂N₂ and drastic increase in conductivity by the presence of Pt clusters. We also mention a large scale synthesis of Fe₃Co alloy inside the melamine-derived N-rich GTs, which shows outstanding oxygen reduction reaction activity with high power density of 117 mW cm⁻² as a cathode material in an alkaline anion exchange membrane fuel cell [Adv. Energy Mater. 2018]. Finally, we address the GNR based 2D-MES, DNA finger printing as well as electronic/spintronic devices [Nat. Nanotech. 2008; 2011; ACS Nano 2014; J. Phys. Chem. Lett. 2016].

Symposium : **KCS2-1**

[KCS-Chemical Industry Joint Symposium] Frontiers in Organometallic Catalysis

Room 322, WED 15:10

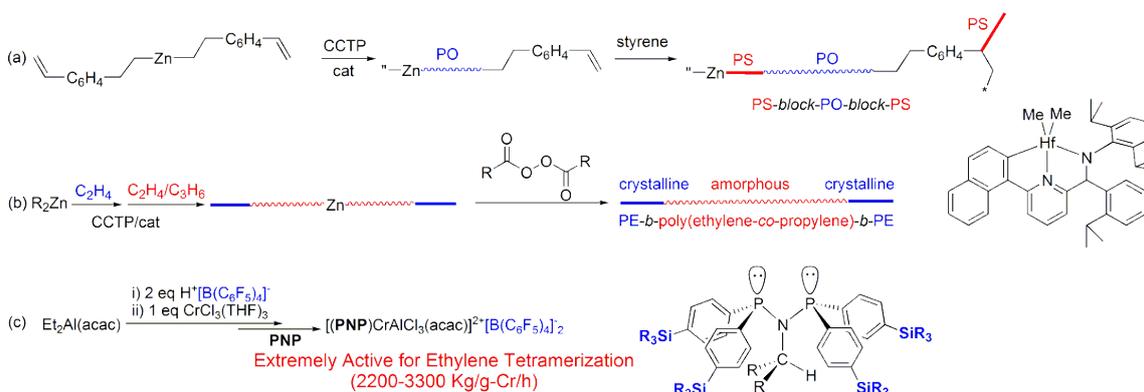
Chair: Ilgu Jung (Chemistry Lab, SK innovation)

Organometallic catalysts for polyolefin industry

Bun Yeoul Lee

Department of Molecular Science and Technology, Ajou University, Korea

Triblock copolymers of polystyrene (PS) and polyolefin (PO), e.g., PS-block-poly(ethylene-co-1-butene)-block-PS (SEBS), are attractive materials for use as thermoplastic elastomers, and are produced commercially by a two-step process, which involves the costly hydrogenation of PS-block-polybutadiene-block-PS. I will present a one-pot strategy for attaching PS chains to both ends of PO chains to construct PS-block-PO-block-PS directly from olefin and styrene monomers (Scheme a). A practical and simple method for the preparation of ABA-type olefin triblock copolymers, e.g., PE-b-poly(ethylene-co-propylene)-b-PE will be presented. been described (Scheme b). The original Sasol catalytic system for ethylene tetramerization is composed of a Cr source, a PNP ligand, and MAO (methylaluminoxane). The use of expensive MAO in excess has been a critical concern in commercial operation. An extremely active catalytic system that avoids the use of MAO will be presented.



Symposium : **KCS2-2**

[KCS-Chemical Industry Joint Symposium] Frontiers in Organometallic Catalysis

Room 322, WED 15:55

Chair: Ilgu Jung (Chemistry Lab, SK innovation)

Microporous Organic Networks and Their Applications

Seung Uk Son

Department of Chemistry, Sungkyunkwan University, Korea

Microporous organic networks (MONs) are a recent class of porous materials. The MON materials can be distinguished from COF or MOF by their amorphous nature and actually, are close to cross-linked polymer. Due to their high surface areas and chemical stability, the MON materials have been applied for various purposes. This presentation will introduce the engineering and chemical functionalization of MON materials. In addition, this presentation will introduce the applications of MON materials.

First, the MON materials have been engineered for the environmental purposes such as removals of particulate matters and Cr(VI) species and for the sensing of harmful targets. Second, the MON materials have been applied for the engineering of battery or supercapacitor materials. Third, The MON materials could be applied for the development of heterogeneous catalysts. Fourth, the MON materials have been utilized for the engineering of drug delivery materials.

Symposium : **KCS2-3**

[KCS-Chemical Industry Joint Symposium] Frontiers in Organometallic Catalysis

Room 322, WED 16:40

Chair: Ilgu Jung (Chemistry Lab, SK innovation)

Hybridization of Metal-Organic Frameworks and Nanomaterials for Gas Storage and Catalytic Conversion

Kyung min Choi

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

Metal-organic frameworks (MOFs) are typically synthesized into pure and bulk-sized crystals, and thus their usability is limited by the lack of compatibility with advanced technologies. Strategies to intermingle reticular chemistry and nanotechnology will lead to new forms of functional materials and applications. This talk will show how MOFs and nanomaterials can be combined into special constructs and successfully work together for heterogeneous and photo-catalysis, and gas separation. In the heterogeneous catalysis, we show how Pt nanocrystals can be fully embedded within single crystals of nMOFs with full control over the size and location of the Pt and MOF nanocrystals. We find that this new (Pt ⊂ nMOF) nanocrystal construct is capable of carrying out the gas-phase conversion of methylcyclopentane (MCP) to acyclic isomer, olefins, cyclohexane, and benzene. These conversions occur at 100 °C lower and with higher selectivity to C6-cyclic products compared to the reference catalyst, and also show that physical and chemical environments of nMOFs control the selectivity and activity to those products. In the photocatalysis, the photocatalytic MOF is prepared by incorporating photoactive molecules and combined with Ag nanoparticles having plasmonic enhancement to make high efficiency and stable CO₂ conversion reaction under visible light. In gas storage, we show that the synthetic methods which combine the optimization for crystal formation with the introduction of heterogeneous structures within a MOF enhance the gas storage properties. In the last part of this talk, we will show our concept and approaches of ppm-level gas storage and catalytic conversion in air for solving many issues about volatile organic compounds.

Symposium : **KCS3-1**

[KCS-Chemical Industry Joint Symposium] Thermo Fisher Technical Academia

Room 306A, FRI 09:00

HPLC Method Development and Introducing Accucore column

Jung Woo Lee

Thermo Fisher Scientific, Korea

For effective HPLC analysis, develop methods of analysis by changing the mobile phase.

Users consider various factors for effective mobile phase design.

Introduce the meaning of various factors such as selection of organic solvent, pH of mobile phase, selection of buffer type, and basic methods for making optimal mobile phase in reversed phase mobile phase.

Also introduce column selection, a key element in the analysis, and the Accucore column of Thermo, which is a popular solid core column.

Symposium : **KCS3-2**

[KCS-Chemical Industry Joint Symposium] Thermo Fisher Technical Academia

Room 306A, FRI 10:00

Vanquish; Innovation of UHPLC

Junghyang Lee

Thermo Fisher Scientific KOREA, Korea

Thermo Scientific's high-end UHPLC system, Vanquish (Horison and Flex), meets the needs of modern lab laboratories by providing optimal resolution and reproducibility results.

In chromatography analysis, the introduction of high pressure UHPLC systems along with the appearance of column of 2um or less are widely used in various fields with improved resolution and sensitivity.

For maximum performance in UHPLC systems, the Vanquish system can withstand the highest pressures of 22,000 psi, while the Smart injection method ensures optimum reproducibility in high pressure systems. Column ovens also provide temperature control in multiple modes to maximize the resolution of the UHPLC. In addition, the introduction of Vanquish DAD detector with Light Pipe Technology makes it suitable for detecting impurities.

The presentation will cover the evolution of UHPLC in separation analysis and the impact of the best Vanquish HPLC system on analyst data quality.

Symposium : **KCS3-3**

[KCS-Chemical Industry Joint Symposium] Thermo Fisher Technical Academia

Room 306A, FRI 10:30

Orbitrap Technology

Scott Peterman

Thermo Fisher Scientific, United States

The unique architecture of Orbitrap™ Tribrid™ mass spectrometers enables novel, powerful data acquisition methods to advance research. The combination of the quadrupole, Orbitrap, and dual pressure linear ion trap mass analyzers along with the ion routing multiple maximizes duty cycle, sensitivity, and selectivity to enable characterization and quantification of complex samples for both small and large molecule studies. In addition, detection in the Orbitrap enables ultra-high resolution and mass accuracy further differentiating instrument performance. Additional method and software features complete the workflow for automated data acquisition and processing.

The presentation will cover the new and unique acquisition methods for small molecule unknown identification and characterization as well as improved proteome coverage using bottom-up and top-down workflows. The presentation will highlight the AcquireX acquisition method as well as Compound Discoverer and Mass Frontier software used to acquire and process MS_n data. For proteomics support, introduction of the FAIMS Pro interface to the Orbitrap Fusion Lumos Tribrid mass spectrometer has significantly increased the proteome coverage compared to data acquisition without FAIMS or TOF mass spectrometers. Proteomics support using the Tribrid mass spectrometer is also enhanced for top-down and in tact analysis.

Symposium : **KCS4-1**

[Presentation by Ministry of Science and ICT] The 2019 Provisional Operation Plans of the Basic Research Programme in the Science and Engineering Field

Room 306B, FRI 11:00

Chair: Lee Yong-Hoon (NRF)

Presentation on “The 2019 Provisional Operation Plans of the Basic Research Programme in the Science and Engineering Field”

Juwon Lee

Basic Research Promotion Division, Ministry of Science and ICT, Korea

The Ministry of Science and ICT under the newly established Moon Jae In Administration will be informing researchers on the 4th Comprehensive Plan for the Promotion Basic Research ('18~'22). It further attempts to listen to researchers' opinions on the operation plans of the basic research programme in the science and engineering field.

Under the Moon Administration's Researcher-Led Basic Research Budget Expansion Policy, the Ministry of Science and ICT plans to boost the basic research programme budget for 2019, and also attempts to reform the programme with researchers as the center.

The major future directions will focus on enhancing funds and providing foundations for new researchers, expanding funds for projects considering efficiency and diversity, and improving research sustainability etc.

Symposium : **KCS6-1**

[Elsevier Lunch Seminar] Making Compounds: A Brief History of and an Outlook into the Future of Synthesis

Planning

Room 325A+B, THU 12:00

Making compounds: a brief history of and an outlook into the future of synthesis planning

Jürgen Swienty-Busch

Elsevier, Germany

Making compounds is an artwork, which requires a lot of experience and knowledge and is at the heart of what chemists do on a daily basis. This talk will demonstrate past and future approaches to support chemists in this challenging task.

Symposium : **KCS7-1**

[Lab Safety Education] Laboratory Safety Education for the Graduate Students

Room 315, FRI 09:00

Chair: Ik Mo Lee (Inha University)

The safety manual for organic chemist and laboratory

Hyunjin Kim

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

This is a safety management education prepared by the Korea Research Institute of Chemical Technology (KRICT). We will analyze the cases of accidents that may occur in the organic chemistry laboratory and how to prevent them. This presentation is aimed at graduate students and researchers who start the research. The topics are safety rules to be followed before the experiment and education and countermeasures to cause accidents by analyzing actual cases of accidents.

Symposium : **KCS7-2**

[Lab Safety Education] Laboratory Safety Education for the Graduate Students

Room 315, FRI 09:30

Chair: Ik Mo Lee (Inha University)

What To Do Prior To Research and Development in Laboratory

Sunyoung Bae

Department of Chemistry, Seoul Women's University, Korea

Conducting experiments associated with research and development in the laboratory requires various processes including material preparation, lab procedures, waste management and so on. It is important to make researchers prepared for these processes before starting an experiment. In addition, laboratory hazard risk assessment in Laboratory Safety Law has been enforced since 2015 to collect basic information about the laboratory, identify and evaluate hazards, and establish safety plan associated with risks. These activities should be achieved by the cooperative efforts between the principal investigators, the researchers, the environment and safety managers, and a head of research institute. This presentation will provide opportunities for the graduate research students and the principal investigators and other related personnel to review the necessary processes prior to starting the experiment associated with research and development in the laboratory and to understand each role toward a culture of safety. Keywords: Laboratory safety, Research and Development Safety Analysis, Hazard, Risk

Symposium : **KCS7-3**

[Lab Safety Education] Laboratory Safety Education for the Graduate Students

Room 315, FRI 10:00

Chair: Ik Mo Lee (Inha University)

Psychology of Accidents and Safety

ChangHo Park

Department of Psychology, Chonbuk National University, Korea

A number of accidents are caused by human error, most of which results from failures in psychological processes such as attention, memory, and judgment. Different kind of human error is involved in various accidents in labs, workplace and everyday situation. Considering different psychological mechanisms underlying human error we can prepare a variety of countermeasures against accidents, concerning environmental design, knowledge and training on safety, communication in workplace, attitude, stress, and so on. Reason's (1984) Swiss cheese model which suggest different levels of failures could provide a good model in understanding accidents and defenses against them. Aspects of risk management are discussed as a final comment.

Symposium : **KCS7-4**

[Lab Safety Education] Laboratory Safety Education for the Graduate Students

Room 315, FRI 10:30

Chair: Ik Mo Lee (Inha University)

Laboratory Safety Act and Laboratory Safety

Ik-Mo Lee

Department of Chemistry, Inha University, Korea

Laboratory Safety Act, registered in April, 2005, has enacted for the safety of researchers in the fields of science and engineering since March, 2006. In this lecture, the background, contents, and recent amendments of this law and recent accident statistics and examples will be presented. The possibility of accident prevention and duties of the research manager will be also discussed.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:00

Chair: Seung Goo Lee (University of Ulsan)

Fluorine-Driven Self-Assembled Polymer Acceptor for Highly Efficient and Flexible All-Polymer Solar Cells

Minjun Kim, Guan-Woo Kim¹, Taewan Kim¹, Junwoo Lee¹, Taiho Park^{1,*}

Chemical engineering, Pohang University of Science and Technology, Korea

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

In this study, a copolymer of naphthalene diimide (NDI) and (E)-1,2-bis(3-fluorothiophen-2-yl)ethene (FTVT) (PNDI-FTVT), which has a low-crystalline structure and high electron mobility, was used as a polymer acceptor. The blend film using PNDI-FTVT exhibited a well-mixed morphology without a large-scale phase separation due to reduced crystalline domain size. In addition, PNDI-FTVT increases intermolecular interactions with the polymer donor by fluorine-driven strong π - π stacking, thereby improving the chain interconnectivity to construct a better charge carrier transport pathway and enhance mechanical resilience in flexible all-polymer solar cells (all-PSCs). PNDI-FTVT based flexible all-PSCs exhibit improved photovoltaic performance compared to PNDI-TVTV based flexible all-PSCs (3.86% \rightarrow 5.90%) as well as excellent mechanical stability, maintaining 72% of its initial performance (5.90% \rightarrow 4.26%). To the best of our knowledge, this is the highest photovoltaic performance for spin-coated flexible all-PSCs and the first report on photovoltaic operation in the bending test.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:10

Chair: Seung Goo Lee (University of Ulsan)

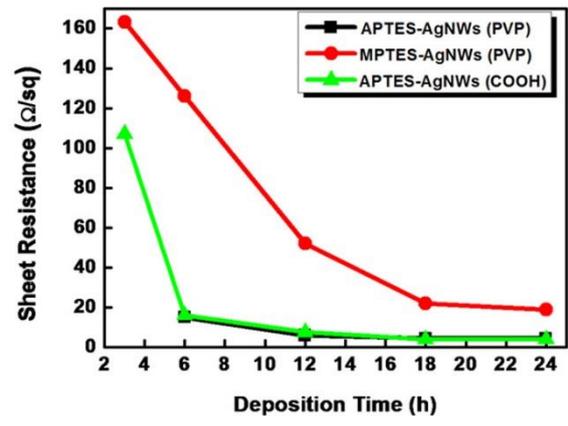
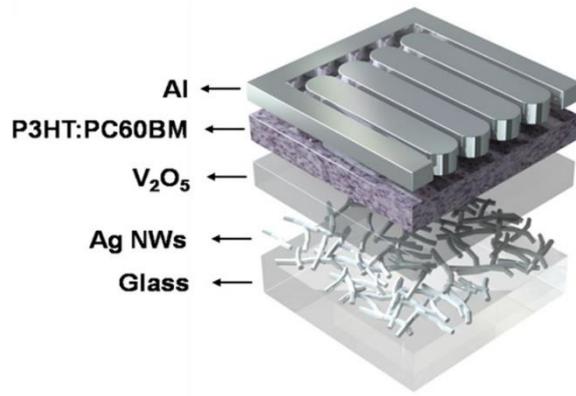
Solution-Processable transparent conducting electrodes via the selfassembly of silver nanowires for organic photovoltaic devices

Heejeong Shin, Hyosung Choi^{1,*}

Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Solution-processed transparent conducting electrodes (TCEs) were fabricated via the self-assembly deposition of silver nanowires (Ag NWs). Glass substrates modified with (3-aminopropyl)triethoxysilane (APTES) and (3-mercaptopropyl)trimethoxysilane (MPTES) were coated with Ag NWs for various deposition times, leading to three different Ag NWs samples (APTES-Ag NWs (PVP), MPTES-Ag NWs (PVP), and APTES-Ag NWs (COOH)). Controlling the deposition time produced Ag NWs monolayer thin films with different optical transmittance and sheet resistance. Post-annealing treatment improved their electrical conductivity. The Ag NWs films were successfully characterized using UV-Vis spectroscopy, field emission scanning electron microscopy, optical microscopy and four-point probe. Three Ag NWs films exhibited low sheet resistance of 4–19 Ω/sq and high optical transmittance of 65–81% (at 550 nm), which are comparable to those of commercial ITO electrode. We fabricated an organic photovoltaic device by using Ag NWs as the anode instead of ITO electrode, and optimized device with Ag NWs exhibited power conversion efficiency of 1.72%.



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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:20

Chair: Seung Goo Lee (University of Ulsan)

Green-solvent processable semiconducting polymers applicable in additive-free perovskite and polymer solar cells: molecular weights, photovoltaic performance, and thermal stability

Junwoo Lee, Guan-Woo Kim, Taewan Kim, Taiho Park*

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

In this study, we demonstrated a novel approach to increase solubility in green solvent (2-methylanisole; food additives) and the effects of the molecular weight (MW) of a green-solvent processable semiconducting polymer (asy-PBTBDT) on its photovoltaic performance and device thermal stability in green processed devices for the first time. The asy-PBTBDT with a high MW (132 kDa) had the highest hole mobility values ($4.91 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ without dopants and $5.77 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ with dopants) as a result of increase in the π - π stacking along with MW as compared to low-MW asy-PBTBDTs (27 and 8 kDa). The high-MW asy-PBTBDT with a high mh achieved the best power conversion efficiencies of 18.2% and 20.0% for the undoped and doped states in PerSCs, respectively, and 5.7% in PSCs in green processed devices. Furthermore, the glass transition temperature increased with an increase in MW; this indicated an effective decrease in heat-induced morphological degradation in the photovoltaic devices. In addition, an increase in the chain density along with MW led to good robustness against humidity and oxygen.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:30

Chair: Jongbok Lee (Texas A&M University)

Biodegradable Shape Memory Polymers: Amino Acid-Based Poly(Ester Urea)s for Biomedical Applications

Gregory Peterson

Chemistry, Seoul National University, Korea

The thermal shape memory behavior of a series of amino acid-based poly(ester urea)s is explored. We demonstrate that these materials exhibit excellent shape memory performance in dual- and triple-shape thermomechanical testing over a range of amino acids and chain extender lengths. The mechanism of shape transformation and recovery is attributed to activation of chain mobility above the glass transition temperature as well as a strong hydrogen bonding network. Additionally, we demonstrate that we can tune the shape memory properties of these materials with polymer blending, enabling quadruple-shape memory cycles. The significance of these findings will be discussed in relation to other biodegradable shape memory polymers and to relevant biomedical applications.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:40

Chair: Jongbok Lee (Texas A&M University)

Redox-Switchable Cross Metathesis and Acyclic Diene Metathesis (ADMET) Polymerization

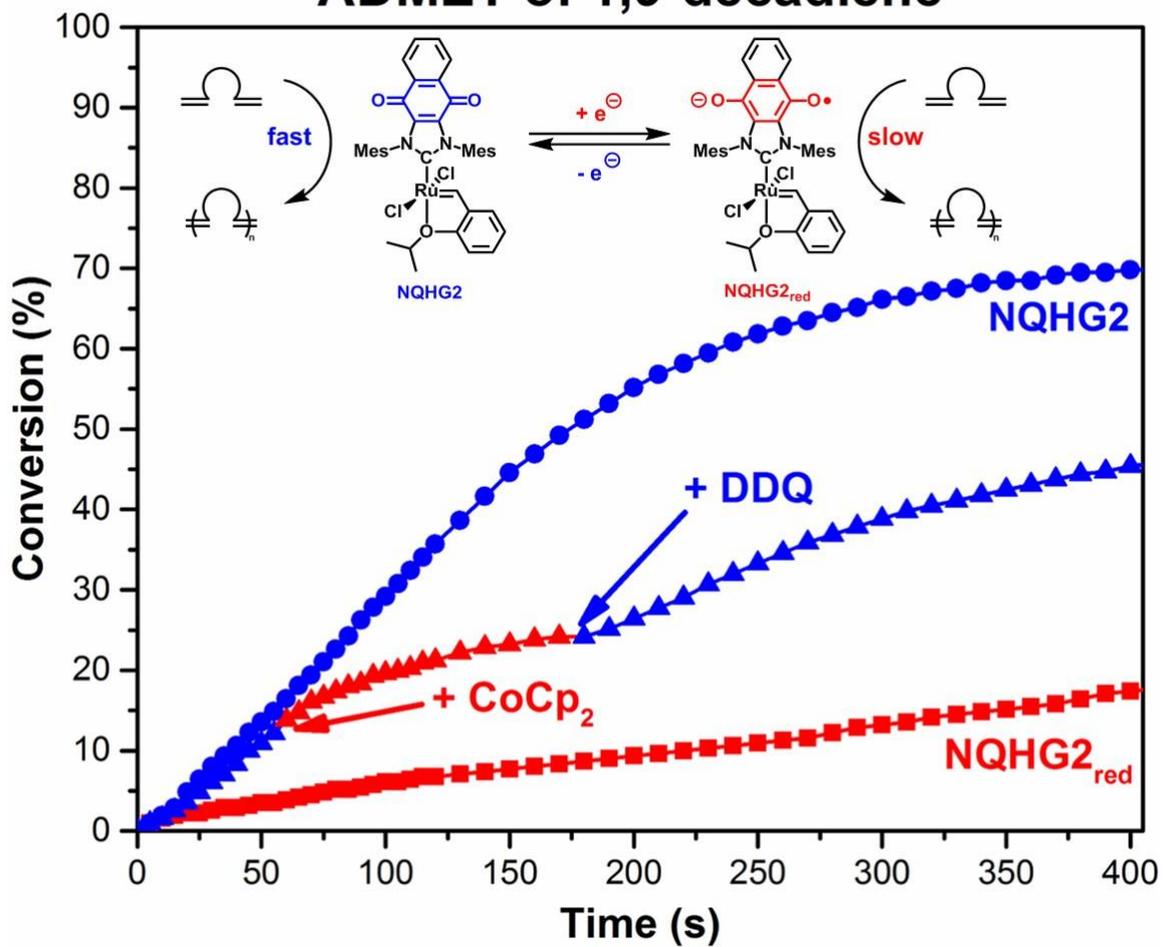
Yeonkyeong Ryu, Christopher Bielawski^{1,*}

Chemistry, Ulsan National Institute of Science and Technology, Korea

¹*Center for Multidimensional Carbon Materials, Institute for Basic Science, Korea*

Acyclic diene metathesis (ADMET) polymerization grant the opportunity to synthesize precisely defined polymers. One of the limitations of this method is the lack of control on the molecular weight of the final products. We reasoned that the use of redox switchable catalysis can be used to achieve enhanced levels of control. Herein, a Ru(II)-based redox-switchable catalyst, containing a quinone-annulated N-heterocyclic carbene is used in order to modulate the reactivity of ADMET polymerization by using redox agents (CoCp₂ and DDQ). The oxidation state of the ligand, switched by reducing and oxidizing agents allow us to control directly the kinetic of the reaction. Whereas the neutral form of the complex catalyzes the reaction (in the same rate as commercially-available catalyst), the reduced complex inhibits the reaction by a decrease in the rate constant by around one order of magnitude, compared to the neutral form. Furthermore, the molecular weight of polymers by ADMET polymerization with this redox-switchable catalysis was related to the same chemistry as mentioned before. In this work we investigate the cross metathesis (CM) reaction because it shares the fundamental mechanism with ADMET polymerization that will be discussed in this work where NQHG2 was used as a catalyst and we will show that is possible to modulate the molecular weights of the final products.

ADMET of 1,9-decadiene



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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 09:50

Chair: Jongbok Lee (Texas A&M University)

Mechanochemical Degradation of the Dendronized Polymers Induced by Ultrasound: Discovering the Link Between Degradation Rate and Polymer Side Chain

Ki-Taek Bang, Gregory Peterson¹, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

¹*Chemistry, Seoul National University, Korea*

Polymer mechanochemistry has attracted much attention since the mechanical force can induce the chemical reaction to the polymer which cannot be initiated by heat, light, electric and chemical reagent. This allows the researchers to develop unique functional materials such as force sensors, self-reinforcing materials. On the other hand, scientists have studied the effect of fundamental properties of the polymers such as polymer architecture on the mechanochemical reactivity. However, there is still a lack of understanding of the mechanochemical behaviours of the macromolecular chain. One of the most important questions is that how does the side chain size affect the mechanochemical response of the polymers. To exploit the side chain effect, we focused on the dendronized polymers bearing well-defined dendritic side chain, which can be tuned at the molecular level by the proper design. In the presentation, I'll describe the synthesis of the dendronized polymer composed of the polyphenylene dendron and their degradation behaviour. The systematic studies using the series of the well-defined dendronized polymers revealed that the size of the side chain affects the degradation rate of the polymers. Moreover, we found the unexpected relationship between the molecular weight of the dendron and the degradation rate. Furthermore, the degradation kinetics and multi-angle laser light scattering (MALLS) analysis showed that the chain extension caused by bulky side chains plays an important role in the mechanochemical response of the polymers.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 10:00

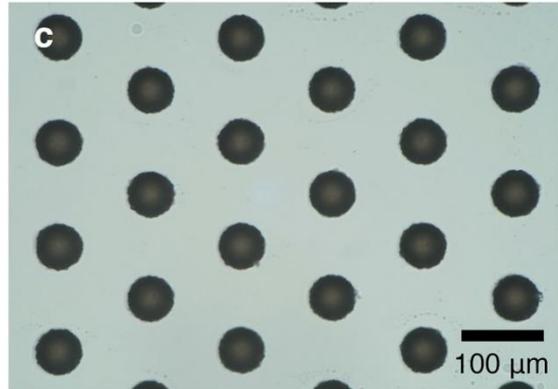
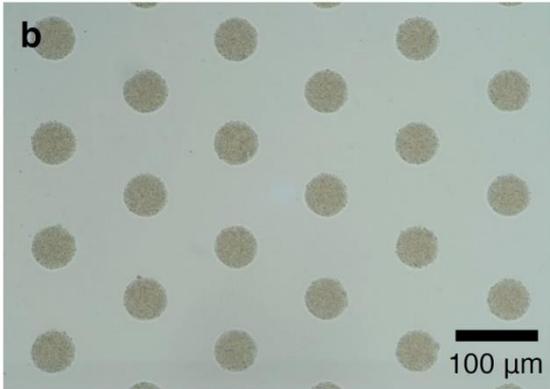
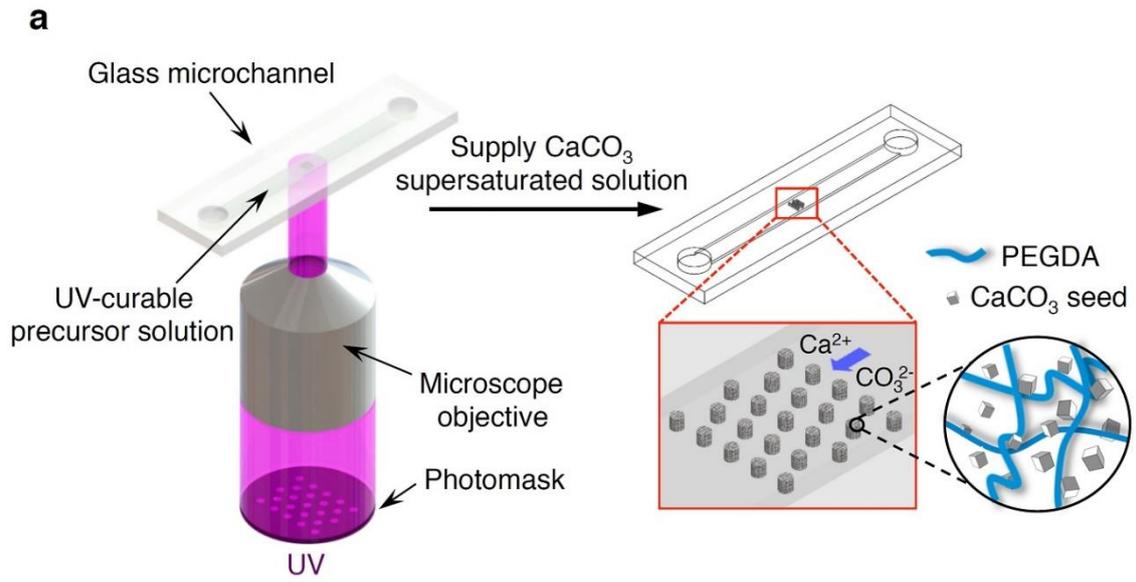
Chair: Younsoo Kim (POSTECH)

Site-Selective In Situ Grown Calcium Carbonate Micromodels with Tunable Geometry, Porosity, and Wettability

Seung Goo Lee

Department of Chemistry, University of Ulsan, Korea

Micromodels with simplified porous microfluidic systems are widely used to mimic the underground oil-reservoir environment for multiphase flow studies, enhanced oil recovery, and reservoir network mapping. However, previous micromodels cannot replicate the length scales and geochemistry of carbonate because of their material limitations. Here a simple method is introduced to create calcium carbonate (CaCO_3) micromodels composed of in situ grown CaCO_3 . CaCO_3 nanoparticles/polymer composite microstructures are built in microfluidic channels by photopatterning, and CaCO_3 nanoparticles are selectively grown in situ from these microstructures by supplying Ca^{2+} , CO_3^{2-} ions rich, supersaturated solutions. This approach enables us to fabricate synthetic CaCO_3 reservoir micromodels having dynamically tunable geometries with submicrometer pore-length scales and controlled wettability. Using this new method, acid fracturing and an immiscible fluid displacement process are demonstrated used in real oil field applications to visualize pore-scale fluid-carbonate interactions in real time.



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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 10:20

Chair: Younsoo Kim (POSTECH)

Extended Ladder-Type Benzo[k]tetraphene-Derived Oligomers

Jongbok Lee, Lei Fang*

Chemistry, Texas A&M University, United States

Ladder-type fused aromatic materials have long been attracted and investigated due to their great electronic and optoelectronic properties with high thermal and chemical properties. In contrast with well-studied pentacene derivatives, which exhibit excellent electronic properties without air stability, constitutionally isomeric benzo[k]tetraphene (BTp) derivatives are stable under ambient conditions and have been barely explored due to the limited synthetic strategy to afford alternating fused rings and extremely low solubility of rigid ladder-type oligomers (i.e. longer than 7-fused rings). Herein, the synthesis of BTp derivatives up to 13-fused aromatic rings was achieved under thermodynamic control by employing reversible ring-closing olefin metathesis. This unique approach featured mild conditions and excellent efficiency, affording a series of BTp derivatives which have not been synthesized before. The good solubility of the BTp derivatives by introducing solubilizing groups at the end of the aromatic rings allowed a rigorous solution-based analysis and feasible processing of thin films using solution-casting techniques. Well-defined BTp systems enabled systematic study of the relationship between chain length and optical properties and effective conjugation length. Moreover, solid-state dynamics of rigid, coplanar BTp derivatives were investigated by grazing-incidence wide-angle x-ray scattering (GIWAXS) and solid-state UV-vis spectroscopy demonstrating the pivotal balance between intermolecular interaction and molecular mobility for optimized processing of highly ordered solids of these extended conjugated molecules.

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

Oral Presentation for Young Polymer Scientists

Room 325C+D, THU 10:40

Chair: Younsoo Kim (POSTECH)

Development of Novel Hole-Transporting Materials for Perovskite Solar Cells via Peripheral Group Engineering

Jaemin Lee

Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea

For the commercialization of perovskite solar cells (PSCs), both high efficiency and long-term stability are required. In a typical n-i-p device configuration of PSCs, organic hole-transporting materials (HTMs) are widely used to transport holes into contact metal. Although a variety of new HTMs for PSCs have been developed so far, enhanced stability as well as enhanced efficiency of PSCs using new HTMs has been rarely reported. In this work, a novel spirobifluorene-based HTM, denoted as DM, was synthesized by altering the peripheries of the very famous Spiro-OMeTAD. At the peripheries of DM, dimethylfluorene was introduced instead of anisole. DM-based PSC device showed certified power conversion efficiencies of 22.6% (~ 0.092 cm²) and 20.9% (~ 1 cm²). As a result of energy level matching between perovskite and HTM, a significant reduction in voltage loss of the photovoltaic device could be obtained. Furthermore, the new HTM, DM, showed the higher glass transition temperature (T_g) than Spiro-OMeTAD, which also resulted in the better thermal stability than Spiro-OMeTAD-based device, maintaining almost ~95% of initial performance for more than 500 h after thermal annealing at 60 °C. Details of our strategy to develop high performance HTMs for PSCs will be discussed in the presentation.

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

Recent Researches of Inorganic Chemists

Room 323, THU 09:00

Chair: Nak Cheon Jeong (DGIST)

Chemical Tools and Tactics 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 β) 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 β plaque and likely contribute to A β neurotoxicity and oxidative stress. ROS have been shown to increase the rate of A β 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.¹⁻⁵ 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 and tactics capable of targeting and regulating its multiple underlying factors simultaneously.²⁻⁴ In this presentation, 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.⁶⁻¹¹

General References
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Award Lecture in Division : **INOR.O-2**

Recent Researches of Inorganic Chemists

Room 323, THU 09:20

Chair: Nak Cheon Jeong (DGIST)

Molecular Biomimetics for Drug Development & Energy Conversion

Jaheung Cho

Emerging Materials Science, DGIST, Korea

Enzymes, responsible for thousands of metabolic processes that sustain life, are macromolecular biological catalysts. Molecular biomimetics is an emerging area where hybrid technologies are developed by using the tools of synthetic chemistry, molecular biology and nanotechnology. In this talk, we will present our recent results on the molecular biomimetics for metal-reactive oxygen species mimicking the active site of O₂ activating enzymes. The metal ions and the supporting ligands are found to be important factors that control the geometric and electronic structures of the metal-reactive oxygen species. Reactivity studies performed with the metal-reactive oxygen species toward external substrates provide mechanistic insight into the active site of metalloenzymes for small molecule activation and/or inhibition. Finally, we are going to introduce our ongoing research at DGIST on molecular biomimetics for medicinal applications and small molecule activation related on the energy conversion.

Award Lecture in Division : **INOR.O-3**

Recent Researches of Inorganic Chemists

Room 323, THU 09:40

Chair: Nak Cheon Jeong (DGIST)

Hexa(2-pyridyl)benzenes for Unique Coordination Chemistry

Eunsung Lee

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

Hexaarylbenzene (HAB) systems have been utilized for developing highly symmetric complexes, which can be applicable to multimetallic complexes, supramolecular materials and metal-organic frameworks (MOFs) for the past decades. Among them, pyridyl derivatized HABs are of great interest due to their ability to coordinate to several metal centers in various binding modes. Nevertheless, rigid and highly symmetric hexa(2-pyridyl)benzene (2-HPB) molecules have not been explored for those interesting applications, possibly due to the synthetic difficulty of hexa(2-pyridyl)benzene. Here we present the synthesis and characterization of 2-HPB and its derivative, and a variety of corresponding coordination complexes with various metal ions including their solution behaviors and luminescence properties. Further potential applications to utilize the coordination complexes of 2-HPB will be discussed.

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

Recent Researches of Inorganic Chemists

Room 323, THU 10:10

Chair: Nak Cheon Jeong (DGIST)

Stimuli-Responsive Molecules and Assemblies: Synthetic Implementation of Minimalist Design

Dongwhan Lee

Department of Chemistry, Seoul National University, Korea

Structure begets function. Novel functions often emerge from novel structures (but not necessarily the other way around), as best exemplified by many shape-adaptive chemical architectures in biological systems. Indeed, a remarkable synergy of individually weak yet collectively strong non-covalent interactions is a recurring theme in both biotic and abiotic molecules and assemblies. Prominent examples include hydrogen bonding and π - π stacking. For some time now, we have been investigating synthetic molecules, in which carbon-based π -conjugation gains extra stability or unusual chemical reactivity by having hydrogen-bonding donor-acceptor groups as part of the delocalized electronic system. In addition to serving as a nice structural template to build in and manipulate light-emitting properties, these molecules allowed entry into "foldable", "stackable", and "non-stackable" (for the sake of fairness) polyaromatics with rational structure design. In this presentation will be discussed the advent, current progress, and broader implications of this chemistry.

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

Recent Researches of Inorganic Chemists

Room 323, THU 10:30

Chair: Nak Cheon Jeong (DGIST)

Porous Coordination Polymers Responding to External Stimuli and Modification of Their Pores for Energy and Environmental Applications

Myunghyun Paik Suh

Division of Chemistry, Seoul National University, Korea

Some porous coordination polymers (PCPs) respond to various external stimuli, which often lead to the structural changes or the chemical reactions of the PCPs, depending on the type of stimuli. In some cases, the structural changes occur with the retention of the single crystal nature, being accompanied with the dynamic movements of the molecular components of the crystals in the orchestral fashion. PCPs have well-defined pores and large internal surface areas, and they have great potentials to be applied in gas storage, gas separation, and electro-catalysis. However, they have intrinsic weaknesses for the practical applications due to low gas storage capacities at ambient temperature, low adsorption selectivity, and non-conducting properties, respectively. To overcome these difficulties and enhance the functionalities of PCPs, we have modified the pore spaces of PCPs by using their responsive nature. In the modification of the pores, we have employed various strategies such as inclusion of specific metal ion guests or organic guests, and fabrication of nanoparticles of metals and metal compounds in the pores. The present lecture will comprise the responsive phenomena of the PCPs, various pore modification methods, and the enhanced functionalities of the resulting PCPs in the energy and environmental applications.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 09:00

Chair: Weon-Sik Chae (KBSI)

Charge transfer at WS₂-SiO₂ interface studied with in-situ photoluminescence imaging

Haneul Kang, Sunmin Ryu*

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

Understanding charge transfer (CT) between two-dimensional (2D) crystals and molecules is important for fundamental research and future applications of 2D material systems. Despite recent surge on this research subject, however, the roles of the interface formed by supporting substrates and their surfaces have not been investigated. In particular, ambient water may form a medium on hydrophilic surfaces for electrochemical reactions with oxygen in the air.[1] In this work, we investigated the CT interaction of single-layer WS₂ with the proposed redox couple of O₂/H₂O serving as a hole dopant.[1] Photoluminescence (PL) and Raman spectra obtained for WS₂/SiO₂ in a gas-controlled optical cell served as an indicator of charge density and showed that hole doping is mediated by O₂ and H₂O. Much reduced CT on hexagonal boron nitride substrates suggested a conclusive role of interface between WS₂ and hydrophilic SiO₂ substrate. Wide-field PL imaging was exploited to investigate spatial inhomogeneity and anisotropy. We will further discuss detailed photophysics of charged excitons (trions) and possible roles of defects in the observed CT reactions. References [1] V. Chakrapani, J. C. Angus, A. B. Anderson, S. D. Wolter, B. R. Stoner, G. U. Sumanasekera, Science 318, 1424 (2007)

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 09:12

Chair: Weon-Sik Chae (KBSI)

Probe-dependent molecular dynamics in heterogeneous mixtures.

Kwang-Im Oh, Carlos Baiz*

Chemistry, University of Texas at Austin, United States

Crowding disrupts solvent hydrogen bond networks and modulates the hydration levels of biomolecules and osmolytes. Although the effect of additives on biomolecular structure and stability has been extensively studied, the role of crowding and heterogeneity is not well understood. Dimethyl sulfoxide (DMSO) is important small organic solvent in adaptable applications, such as protein destabilization, cryopreservation, and drug permeation. In particular, DMSO disrupts the hydrogen-bond networks of water in DMSO/water binary mixtures. Here, vibrational spectroscopy combined with molecular dynamics simulations (MD) and quantum chemistry models was used to describe the mechanism by which H-bond interactions of DMSO/water mixtures and crowding effects these heterogeneous systems. Based on directly quantifying H-bond populations using the S=O stretching vibration of DMSO, we show that crowding stabilizes hydrogen bonding in aqueous DMSO. Specifically, we use formamide and dimethylformamide (DMF) as molecular crowder, and map hydrogen bond populations of the S=O and C=O groups in DMSO/water/formamide or DMF ternary mixtures. Further, we use probe-dependent 2D IR spectroscopy to quantify H-bond solvation dynamics, in binary mixtures. The results are as follows; 1. hydrogen bonds are formed and broken through a “step-in” mechanism, which involves hydrogen bonding between water and the DMSO aggregate species. 2. amide additives increase the amount of water within the DMSO first solvation shell, 3. C=O stretching vibrations sense inhomogeneity and solvation dynamics of binary mixtures at varying concentrations.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 09:24

Chair: Weon-Sik Chae (KBSI)

p- and n-type Doping Effects on the Electrical and Ionic Conductivities of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ Anode Materials

Chiho Lee, Sang Uck Lee*

Department of Bio-Nano Engineering, Hanyang University, Korea

We systematically investigated p- and n-type doping effects on the electrical conductivity of spinel $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO) by designing theoretically stoichiometric $\text{Li}_{11}\text{Ti}_{13}\text{O}_{32}$ (p-type) and $\text{Li}_{10}\text{Ti}_{14}\text{O}_{32}$ (n-type) because LTO has a non-stoichiometric $(\text{Li})_{i8}[\text{Li}_{8/3}\text{Ti}_{40/3}]\text{O}_{32}$ formula with the $\text{Fd}\bar{3}\text{m}$ space group. In this work, we present evidence that the electronic modification plays a fundamental role in the electrical conductivity of LTO, especially, n-type $\text{Li}_{10}\text{Ti}_{14}\text{O}_{32}$, which has superior electrical conductivity compared to p-type $\text{Li}_{11}\text{Ti}_{13}\text{O}_{32}$. We proposed a way to improve the electrical conductivity of pristine LTO by halogen ion doping, $\text{Li}_4\text{Ti}_5\text{O}_{12-x}\text{Hal}_x$ (Hal: F, Cl and Br), for an n-type doping effect. However, the substitution of halogen ions can enhance the electrical conductivity by mixing $\text{Ti}^{4+}/\text{Ti}^{3+}$ and impede the Li ion diffusion in the lattice. The larger size of Cl and Br increases the Li ion diffusion energy barrier with van der Waals repulsion. Therefore, our theoretical investigations of the effects of halogen doping on the electrical and ionic conductivities anticipate that the smaller-sized F may be the most promising dopant for improving the performance of LTO.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 09:36

Chair: Weon-Sik Chae (KBSI)

Excited state intramolecular proton transfers and solvation dynamics probed by femtosecond stimulated Raman spectroscopy

Myungsam Jen, Sebok Lee, Kooknam Jeon, Joonwoo Kim, Yoonsoo Pang*

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

Proton transfer reactions are one of fundamental chemical reactions and have been of great interest in many disciplines including chemistry and biology. Excited state intramolecular proton transfer (ESIPT) of 1,2-dihydroxyanthraquinone (alizarin) and (1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione (curcumin) between a hydroxyl and the adjacent carbonyl occurs on ultrafast time scales (

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 09:48

Chair: Weon-Sik Chae (KBSI)

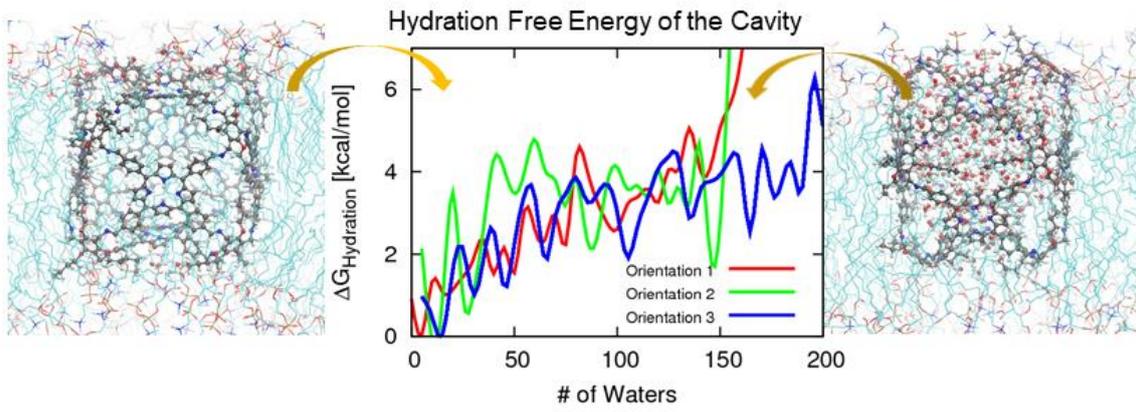
Computational studies of selective anion transport across a porphyrin-based organic cage

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

Selective gating of essential molecules across cellular membrane is one of salient machinery that contributes the homeostasis of living cells. Synthetic transmembrane channels have been designed that can mimic the functionalities of natural channel proteins. These molecule bear a wide variety of applications in biomolecular and medicinal sciences. Recently, the Kim group at IBS/Postech reported a novel porphyrin based covalent organic cage, that can serve as an anion selective channel across cellular membrane. We elucidate the underlying mechanisms of the selective transport based on a set of molecular dynamics (MD) simulations. Long-time MD simulations ($>10 \mu\text{s}$) of the cages embedded in model membranes showed that the internal cavity of the cage undergoes dewetting spontaneously. Umbrella sampling MD simulations showed that the dry state is thermodynamic minimum, whereas the wet states are energetically uphill only by a few kcal/mol that constitute local minimums in energy. These findings suggested that the wet state can occur intermittently, that explain the bursty ion flow observed experimentally. Metadynamics MD simulations of monovalent anions (I^- and Cl^-) confirmed that the wet state allows facile transport of anions and the dry state blocks the permeation. Moreover, we showed that iodide interacts favorably with the alkyl chains attached to the cages, that explains the higher permeability of iodide over chloride. Lastly, we compared the hydration propensities of the metal-free and the Zn(II) bound cages, that suggests a viable strategy to control the wet-dewetting behavior of the cages.



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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 10:00

Chair: Jerome K. Hyun (Ewha Womans University)

Non-equilibrium effect on the kinetics of the polymer loop formation

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Department of Chemistry, Sogang University, Korea

The local equilibrium approximation (LEA) is a fundamental approximation in many theories and studies, however little is known about a measurability of a deviation from local equilibrium or the effect of the breakdown of the LEA on physical properties. Using coarse-grained molecular dynamics simulations, we calculate a rate constant (k_{loop}) of a loop formation reaction by varying a solvent viscosity (η_{sol}) in two types of explicit solvents and investigate the effect of LEA's breakdown on the loop formation kinetics. We find that $k_{\text{loop}} \sim \eta_{\text{sol}}^{-1}$ predicted by celebrated Kramers theory appears where the LEA is satisfied. On the other hand, a fractional viscosity dependence ($k_{\text{loop}} \sim \eta_{\text{sol}}^{-\beta}$, $\beta < 1$) which is a central issue of folding dynamics appears where the LEA breaks down. We suggest the failure of the LEA may contribute to the origin of a fractional dependence of the rate constant on the solvent viscosity. We also show that a mutual information could quantify such deviation from the local equilibrium by capturing an increased correlation due to LEA's breakdown.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 10:12

Chair: Jerome K. Hyun (Ewha Womans University)

Origin of Zundel broadening explained via particular vibrational modes of Eigen structure altered by solvent environmental effects

Yevhen Horbatenko^{*}, Cheol Ho Choi^{*}

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Detailed molecular mechanism of the proton transfer in liquid water has been an intriguing issue, since it plays a crucial role in chemical as well as biological processes. To investigate the dynamics of the proton transfer, ultrafast infrared spectroscopy has been widely used. However, a broad continuous absorption band that appears in a region of $\sim 1800\text{--}3000\text{ cm}^{-1}$ makes interpretation of spectra a challenging task. Many theories have been proposed to interpret the origin of this broadening, but none of them seems satisfactory explains it. Here, ab initio molecular dynamics and instantaneous vibrational mode analysis of various protonated ice as well as water structures have been performed to understand the origin of the broadening in the infrared spectra. Based on the simulations, the origin of the broadening for the first time is explained via contribution from three OH stretching modes of the Eigen structure, i.e., symmetric *A₁* and asymmetric doubly degenerate *E*. The infrared spectrum of the gas-phase Eigen structure (hydronium with the first solvation shell) reveals that these three OH modes fall into one band. As shown, splitting of this band into three, e.g., in ice is caused by the second solvation shell. These bands are further broadened in liquid water due to random motions of the solvent molecules.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 10:24

Chair: Jerome K. Hyun (Ewha Womans University)

Unveiling C1, C2 and C3 mechanism of electrochemical CO₂ reduction at sulfur vacancy of MoS₂: Ab initio study

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Materials Science and Engineering, Seoul National University, Korea

MoS₂ is receiving large attention as a promising electrochemical carbon dioxide reduction (CO₂R) catalyst which shows good selectivity and current density at edge site in ionic liquid [1-3]. Recently, Francis et al. reported that CO₂R is occurred at basal plane of MoS₂ which produces 1-propanol as a major product [4]. In this work, we investigate the catalytic performance of CO₂R at sulfur vacancy (Vs) of MoS₂, which has been recently reported as an active site for HER [5], by density functional theory. Possible reaction paths are investigated by modifying computational hydrogen electrode model as considering charged states of intermediates [6]. We first calculated pathways for C1 product: formic acid, formaldehyde, methane and methanol are identified as possible products at potential of -0.4 V vs RHE. In addition, C2 products (ethanol, ethylene glycol) and C3 products (1-propanol, 1,3-propylene glycol) were possibly evolved at the same potential with C1 products (-0.4 V vs RHE). Our results well explain recent experiment on CO₂R at single-crystal and thin film MoS₂ electrode that 1-propanol is evolved at -0.59 V vs RHE as a major product. Minor products were produced such as formate, ethylene glycol, t-butanol, methanol and methane at the same potential [4] which was also in agreement with our results. Finally, based on verified mechanism, we suggest cascade structure of Vs-MoS₂ with other catalysts, which produces HCHO as a major product, to enhance selectivity of CO₂R vs HER at Vs-MoS₂. [1] Nat. Commun., 2014, 5, 4470.[2] Science, 2016, 242, 467.[3] ACS Nano, 2018, 11, 453.[4] Chem. Mater., 2018, 30, 4902.[5] Nat. Mater., 2016, 15, 48–53.[6] ACS Catal., 2018, 8, 4508.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 10:36

Chair: Jerome K. Hyun (Ewha Womans University)

Effect of Underdamped Vibration on Energy Transfer: Direct Comparison between Two Different Partitioning Schemes

Chang Woo Kim, Young Min Rhee*

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

In this work, we studied excitation energy transfer (EET) in a model three-site Frenkel exciton Hamiltonian embedded in phonon environment. The reduced density matrix of the quantum subsystem was simulated by using a mixed-quantum classical dynamics method, which treats the environment as a collection of classical nuclei. We mainly focus on the effect of underdamped vibration, which is included either in the environment or in the quantum subsystem. For both cases, we observed that EET is boosted when the frequency of vibration mode matches the electronic energy gap. This demonstrates that intricate features of EET dynamics that have been frequently ascribed to arising with quantal vibrations, such as electronic-vibrational mixing, can be successfully reproduced by using physically equivalent but classically described bath modes. We will explain the origin of this quantum-classical correspondence based on the non-equilibrium relaxation in the electronic excited states. Finally, we will also discuss how the effect of bath modes on EET dynamics depends on their timescale of fluctuations.

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

Oral Presentation for Young Scholars in Physical Chemistry

Room 324A, THU 10:48

Chair: Jerome K. Hyun (Ewha Womans University)

Ultrafast measurement of transient absorption and refraction spectra with frequency comb in femtosecond to nanosecond time window

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¹Department of Chemistry, Korea University, Korea

Transient absorption (TA) is the most widely utilized time-resolved spectroscopy technique for studying various photochemical reactions. Basically, TA is a pump-probe type experiment that a probe monitors the changes in spectral response induced by a pump with varying the optical time-delay between the pump and probe, T . Typical TA experiment controls T by a mechanical translational stage, while a dispersive spectrometer records the probe spectrum at each T . Recently, we developed dual frequency-comb (DFC) based interferometric pump-probe spectroscopy (DFC-IPS). DFC is consisted of two mode-locked lasers with highly stable two frequency degree of freedoms, repetition rate and carrier-envelope-offset frequency. By detuning the repetition rates of two lasers, which act as a pump and probe lasers, it is able to scan T linearly and automatically. The automatic T -scan is advantageous to study long-lasting dynamics because it preserves the spatial beam quality regardless of T . DFC-IPS can record a two-dimensional TA and transient refraction spectra with broad frequency (650 nm to 950 nm) and time window (12 fs to 10 ns) just in few seconds. Additionally, DFC-IPS data is simply measured by a single photodetector. This provides the capabilities for the experiments requiring parallel data acquisition, such as anisotropy and chirality measurement. These peculiar properties of DFC-IPS, the absence of mechanical T -scan and the use of single detector, make the experimental setup simpler than the typical TA experiment. Finally, a gated sampling is available in DFC-IPS, so that easily damageable photochemical reaction systems can also investigated.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:00

Chair: Tae-Young Kim (GIST)

Development and application of selective and sensitive fluorescence-labeling for analysis of proteins distribution in food

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Department of Chemistry, Hannam University, Korea

¹*Department of Food Technology, Engineering and Nutrition, Sweden*

Proteins play important fundamental roles in food derived from plants and animals with their nutritional, emulsifying and many other functional properties^[1]. Gum Acacia (GA), a type of exudate gums obtained from trees of the Acacia species, is widely used as a protective colloid and an emulsifier in food and drink. The emulsification property of GA is known to be influenced by the protein content, and is usually reduced by eliminating protein components^[2]. Determination of the protein content and its distribution in food is thus of great interest. Sometimes the protein content in food is low, and development of a selective and sensitive method for protein analysis is needed. In this study, 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC)-dye fluorescence labeling method was developed for analysis of protein in relatively lower content. GA was separated and characterized by asymmetrical flow field-flow fractionation (AsFIFFF) coupled online with multi-angle light scattering (MALS), differential refractometer (dRI) and fluorescence detector (FL), AsFIFFF-MALS-RI-FL, which yielded molar mass, size, protein content and its distribution in GA. Results showed that the EDC-labelling allows highly sensitive and selective analysis of proteins in food samples of low protein contents. Both the labeling efficiency and the reaction rate increased as pH increased from 7 to 11. The AsFIFFF-MALS-dRI-FL provides a powerful characterization tool for protein-containing food samples.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:10

Chair: Tae-Young Kim (GIST)

Development of iCLEM for real-time observation and easy sample replacement.

GwangHoon Lee, Boklae Cho^{1,*}

Charged Particle Beam Research Institute, ModuleSci Co., Ltd., Korea

¹*Korea Research Institute of Standards and Science, Korea*

Quantum dots and light emitting diodes (LEDs) are normally studied by using a light / fluorescence microscope (LM / FM) due to their luminescent properties. However, when a problem occurs in a device, the defect is often much smaller than a micron, making it difficult to identify its origin with a general light microscope. To overcome these limitations, an electron microscope with higher resolution than a light microscope should be used. The CLEM (Correlative Light and Electron Microscope) is a device that allows a sample holder to be shared by two microscopes and can perform high magnification imaging using an electron microscope. However, the sample can be deformed or contaminated during the transportation of the holder between the equipments. In order to overcome these drawbacks, various attempts have been made to develop an iCLEM (integrated CLEM). We have developed two kinds of iCLEM consisting of an upright type and an inverted type, maximizing system scalability and accessibility. The upright iCLEM can acquire light / fluorescence images and scanning electron microscope images of an optically opaque sample simultaneously by using a light mirror with a center hole. The inverted iCLEM can image an optically transparent nano-bio sample through a sample holder where the sample is loaded on ITO (Indium Tin Oxide) coated glass. The iCLEM can acquire fluorescence information. We are now constructing a platform that combines iCLEM with EDS, Raman spectroscopy, and CL (Cathode-Luminescence) detector. In this presentation, we will discuss the principles and structure of the iCLEM and show the images to discuss future applications.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:20

Chair: Tae-Young Kim (GIST)

Understanding mechanism of axially perpendicular offset scheme for minimization of glass background in the spectra of housed samples in glass bottles by Monte-Carlo simulation

Duy Pham Khac, Tung Vu, Yoon Jeong Lee, Eunjin Jang¹, Hoeil Chung*

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¹*Chemistry, Hanyang University, Korea*

When a laser beam is irradiated on a side of a sample-containing glass bottle, the generated glass Raman photons are expected to be more localized near the wall, while Raman photons of the sample are more widely distributed throughout the bottle. Interestingly, since bottom of a glass bottle is usually curved, it would be possible to generate conical-shaped field-of-view (FOV) for Raman photon detection, which would be beneficial to separate the localized glass Raman photons near the bottle wall from the wide-spread sample photons. In this case, axially perpendicular offset (APO) scheme incorporating an axially perpendicular geometrical arrangement between laser illumination and photon detection would be as a versatile tool for minimization of contributions of glass background in direct measurements of Raman spectra of samples contained in glass bottles. By using APO scheme, with a longer offset distance between laser illumination spot and detection; it could help further the FOV from localized glass Raman photons near the bottle wall and isolating the glass signal. In this study, Monte-Carlo simulation was applied to explain and visualize the mechanism of minimizing glass background in APO measurements by simulation Raman photon distribution in the samples. The FOVs for Raman photon detection were measured experimentally and simulated accordingly in each case. The results of this simulation were found to be accordant with the experimental observations.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:30

Chair: Tae-Young Kim (GIST)

The role of electrophilicity with substituted para-thiophenols in Surface-Enhanced Raman Scattering

Minjung Seo, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Surface-Enhanced Raman Scattering (SERS) is considered an important analytical technique that has two main mechanisms : the electromagnetic effect related with the localized surface plasmon resonance (LSPR) of nanoparticles and the chemical effect connected with charge-transfer between nanoparticles and probe molecules. In chemical effect, the probe molecules play an main role via the chemical bonding with nanoparticles and there is much potential to find unrevealed regions to elucidate SERS mechanism completely. To understand the relationship between the electrophilicity of molecules and SERS enhancement focused on the chemical effect, para-substituted thiophenols derivatives with strong gold-sulfur interaction and gold nanorods (AuNRs) on resonance condition are chosen. We study SERS behaviors following the electrophilicity of substituent, such as electron withdrawing group (EWG) and electron donating group (EDG), in self-assembly monolayers (SAMs) system and reveal that stronger EWG groups show higher enhancement supporting our assumption that EWG propably promotes a charge-transfer in SERS.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:35

Chair: Tae-Young Kim (GIST)

A simple laser-induced breakdown spectroscopy analysis method for Mg and Ca in edible salts: Sample surface height optimization and intensity normalization

Kim Hyang, Yoonji Jeon¹, Wonbae Lee, Sang-Ho Nam, Yonghoon Lee*

Department of Chemistry, Mokpo National University, Korea

¹Mokpo National University, Korea

Feasibility of a simple laser-induced breakdown spectroscopy (LIBS) instrument has been investigated for analysis of Mg and Ca in edible salts. The LIBS instrument was assembled with a compact low-power diode-pumped solid-state laser and a non-gated handheld spectrometer. A simple sampling process, called a dip-and-dry method, was employed for on-site application; a piece of filter paper was dipped in aqueous solution of the sample salt and dried to be analyzed by LIBS. The analytical performance could be significantly improved by (i) optimization of the sample surface height during laser ablation and (ii) normalization of the analyte line intensities using the Na I line at 616 nm as a reference signal. For commercially available salt products, the Mg II and Ca I line intensities could be well correlated with the concentrations of Mg and Ca determined by inductively coupled plasma- optical emission spectroscopy. Our results indicate that the combination of a compact low-cost LIBS device and the simple sampling method is promising as an on-site salt quality monitoring methodology.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:40

Chair: Tae-Young Kim (GIST)

Profiling of lipoproteins from postmenopausal patients with osteoporosis by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

Kang geun Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Pathological mechanism of osteoporosis is unknown, but osteocytes affected by oxidized lipids inside the body have been known as a major factor. Bone mineral density (BMD) reaches at a highest level in mid 30s and decreases slowly over time, meaning that symptoms are hard to be detected and already serious when found out. Lipids play important roles in signal transmission, cell formation, and various cellular processes and they are expected to be biomarkers of a number of diseases. Therefore, it is interesting to study relationships between lipids consisting lipoproteins in plasma and osteoporosis for early diagnosis. There are several studies about lipids and osteoporosis in the medical field which BMD showed a positive correlation with low-density lipoprotein (LDL) and an inverse correlation with high-density lipoprotein (HDL). However, none of them conducted quantitative and qualitative analysis at the molecular level in detail. In this study, 39 plasma samples of woman were classified into three groups of patients in which women having osteoporosis with no clinical history (n=10), women having osteoporosis with history (n=7), age-matched control (n=22). Lipoproteins were first separated by sizes using asymmetrical flow field-flow fractionation and then lipids contained in HDL and LDL were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS).

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:45

Chair: Tae-Young Kim (GIST)

Effect of adsorbate electrophilicity and sharp tips on single gold nanobipyramids.

Geunwan Kim, Ji Won Ha*

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Gold nanoparticles behave as strong absorbers and scatterers because of localized surface plasmon resonance (LSPR) which is coherent oscillation of conduction electrons at the surface of plasmonic nanoparticle stimulated by the electromagnetic field of incident light. The LSPR peak shift is caused by changes in the medium dielectric constant. However, our understanding of the effects of electrophilicity of thiol molecules adsorbed on gold nanoparticle surfaces is still unsatisfied. In this study, we present dark-field (DF) scattering studies on electrophilicity effect of adsorbate molecules with real time measurement at the single particle level. We found that LSPR wavelength of the gold nanobipyramids (AuBPs) was red-shifted as thiol molecules were adsorbed onto their surface. The electrophilicity of adsorbate molecules was strongly affected to degree of red-shift. Furthermore, the red shift of LSPR wavelength of single AuBPs were rapidly saturated in real-time measurement. This result indicate that AuBPs are highly sensitive to thiol molecules because of the sharp tips and can be used to develop highly sensitive LSPR biosensors.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:50

Chair: Tae-Young Kim (GIST)

Separation of lipoproteins and exosome in plasma using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Lipoproteins transport hydrophobic molecules such as cholesterol in blood and are known to be associated with diseases such as arteriosclerosis. Lipoproteins are classified by high-density lipoprotein (HDL, 5~15 nm), low-density lipoprotein (LDL, 18~28 nm), very low-density lipoprotein (VLDL, 30~80 nm) according to its size and density. Exosomes are extracellular vesicles secreted by cells and their sizes are known as about 30~150 nm in diameter, which are larger than LDL but similar or slightly larger than VLDL. Exosomes are known to play an important role in the intercellular communication as a mediator of RNA, protein, and lipids, therefore, it can be expected to be utilized for disease prognosis and treatment. However, the separation of lipoproteins and exosomes from blood has not been studied extensively. Field-flow fractionation (FFF) is capable of separating sample components from nano to micron size. In this study, lipoproteins and exosomes from blood plasma samples were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) using field programming and detected by UV spectrophotometer (UV) and multi-angle light scattering (MALS). After separation and fractionation by FI-AF4, lipoproteins and exosomes were confirmed by Western blot and transmission electron microscope (TEM).

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 09:55

Chair: Tae-Young Kim (GIST)

Accurate determination of total arsenic in rice considering arsenic species

Wonbae Lee, Ngo Van Tho, Sang-Ho Nam*

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Accurate determination of arsenic in a sample has been important because the toxicity related to the arsenic element has been widely known. In particular, arsenic species must be well considered because their toxicity varies according to chemical form. If the total arsenic in a sample is in trace level below the allowance maximum of any arsenic species, the quantitation of total arsenic might be satisfactory. In general, for the quantitation of total arsenic in a sample, arsenic species in a sample have been not considered at all. The standard solution of total arsenic has been made by As⁵⁺ standard solution. It might be good for the sample which its major species are As⁵⁺. But, if the major species of arsenic in a sample are different from As⁵⁺, the standard arsenic species for calibration curve must be deeply considered. This study showed the amount of total arsenic in a sample could be falsely obtained by the standard solution of different arsenic species. The standard arsenic species used in this study were As³⁺, As⁵⁺, MMA, DMA and AsB. Total arsenic was analyzed in rice using various methods including standard addition method and internal standard method. Ge, In, Rh, Te and Se as internal standards were also investigated for the determination of total As in rice. The best internal standard for total arsenic in rice was Te.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:00

Chair: Tae-Young Kim (GIST)

Simultaneous Determination of 39 Steroid Hormones in Human Urine Sample Using Liquid Chromatography-electrospray Tandem Mass Spectrometry

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²*Center for Chemical Analysis, Korea Research Institute of Chemical Technology, Korea*

Abnormal production or metabolism of steroid hormones are responsible for the development and prevention of endocrine diseases. Accurate quantification of steroid hormones is necessary for both research into clinical conditions as well as for diagnostic monitoring. In this research, an improved analytical method was developed using liquid chromatography-tandem mass spectrometry (LC-MS/MS) for the analysis of 39 steroid hormones including corticosteroids, progestins, estrogens, and androgens in urine sample. As a pre-treatment procedure prior to LC-MS/MS analysis, hydrolyzation of the human urine samples with β -glucuronidase and solid-phase extraction for purifying the samples was performed. Steroids were separated using Waters ACQUITY @ BEH C₁₈ column (2.1 x 100 mm, 1.7 μ m) and a mobile phase consisting of eluent A (0.01% formic acid and 1 mM ammonium formate in water) and eluent B (0.01% formic acid and 1 mM ammonium formate in methanol) with a gradient program at a flow rate of 0.4 mL/min. The [M+H]⁺, [M+NH₄]⁺ and [M+H-H₂O]⁺ ions were used as precursor ions to detect endogenous steroid hormones in MS. All steroids were monitored in multiple reaction monitoring (MRM) mode within 30.0 min by tandem mass spectrometry (MS/MS) with electrospray ionization in positive mode. The linearity of this method was over 0.991. The limits of detection at signal to noise (S/N) ratio of 3 were 0.1 ~ 300 ng/L. The coefficients of variation were in the range of 2 -25% for within-day variation and 2 -25% for day-to-day variation, respectively. The present method could be applied to clinical research such as diagnosis, monitoring, and biomedical investigations.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:05

Chair: Tae-Young Kim (GIST)

Highly sensitive molecular diagnostics using SERS-PCR

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Recently, quantitative real-time PCR (QPCR) have been extensively used for the diagnosis of a wide range of infectious diseases. This technique found valuable clinical application in the diagnosis of viral diseases. However, QPCR suffers from several problems including time-consuming process and high fluorescent background signal. In the present work, we developed a novel molecular diagnostic method using SERS-PCR for the sensitive and specific detection of target genes. Due to the characteristics of amplifying Raman signals by factors up to 10-14 orders of magnitude and unique molecular fingerprinting information, surface-enhanced Raman scattering (SERS)-based biosensors provide ultrahigh sensitivity and have more advantages over the fluorescent detection method. In the present study, we employed an asymmetric-PCR to amplify the target gene in a short time, and then a SERS detection technique has been used for its highly sensitive detection. By combining the PCR and SERS as a detection tool, it would prove to be effective for the rapid and sensitive detection of a low concentration of target. References 1.Kneipp, K., Wang, Y., Kneipp, H., Perelman, L. T., & Itzkan, I, Phys. Rev. Lett. 78, 1667 (1997).2.Wu, Y., Jiang, T., Wu, Z., & Yu, R, Biosens. Bioelectron, 99, 646-652 (2018).Keywords: SERS-PCR, Pseudomonas aeruginosa, Ratiometric gene detection, molecular diagnostics

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:10

Chair: Tae-Young Kim (GIST)

NMR-based urinary profiling reveals different metabolic patterns in focal segmental glomerulosclerosis and minimal-change disease

Jin Seong Hyeon, Geum-Sook Hwang*

Korea Basic Science Institute, Korea

Focal segmental glomerulosclerosis (FSGS) and a related disorder, minimal-change disease (MCD), are idiopathic glomerular disease related to podocytopathies. Although the renal biopsy is mandatory to confirm the diagnosis and guide therapeutic plans in patients with FSGS and MCD, biopsy is an invasive procedure affected by complications. We performed NMR-based urinary metabolic profiling analysis to investigate metabolic differences between FSGS and MCD. The PCA scatter plot showed a clear separation between FSGS and control groups. Moreover, MCD groups were slightly separated from FSGS groups. The significant metabolic alteration in FSGS and MCD groups compared to healthy control groups were related to tricarboxylic acid cycle, choline, and branched chain amino acid metabolism. Furthermore, metabolite that are significantly altered in the FSGS groups included alanine and lactate, whereas MCD groups contained 3-aminoisobutyrate. This study demonstrates that metabolic profiling is useful for understanding metabolic differences between FSGS and MCD patients, and diagnosing kidney disease.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:15

Chair: Tae-Young Kim (GIST)

Alteration of plasma lipidome among five representative cancers by nUHPLC-ESI-MS/MS

Gwang Bin Lee, JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Cancer is one of the critical social problems as the incidence grows every year. Causes of cancer are known to be genetic factors, regimen, and environment conditions and so on. Because of the complexity of the cause, it is very important to understand the cause of cancer more clearly. Lipid is one of the substances that play key roles in the metabolism of human bodies and also known to be associated with various cellular processes such as survival, proliferation, and death. These cellular processes are associated with cancer genesis pathways, especially to transformation, progression, and metastasis, suggesting that lipids are mediators of carcinogenesis processes. In a recent research, lipidomic analysis as regard to cancer attracts more interests since each type of cancer has different carcinogenesis pathways and characteristics. In this study, plasma lipids from 5 different types of cancer patients (liver, gastric, lung, colorectal, and thyroid cancers) were investigated in order to figure out lipids that show significant differences among the groups and to find potential lipid biomarkers of each cancer. Lipids were extracted from blood plasma sample using the modified Folch method with MTBE/methanol, and analyzed by nUHPLC-ESI-MS/MS. Overall, 357 lipids from patient's plasma with liver, stomach, lung, colorectal, thyroid cancer, and controls, were identified and 242 lipids were quantified by nUHPLC-ESI-MS/MS with statistical evaluations for the selection of candidate biomarkers.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:20

Chair: Tae-Young Kim (GIST)

An Synthetic Approach to Si/N-Doped Graphene Quantum Dots Nano-Architecture as anode for Li secondary batteries

Hasan Jamal, Jin-Yeong Choi, Chang-Seop Lee*

Department of Chemistry, Keimyung University, Korea

Despite the pulverization and unstable solid-electrolyte interface (SEI) challenges, silicon is yet a promising high capacity anode material because of its high gravimetric capacity (~4200 mAh/g). Advancements in nano-architecture Si electrodes still remain a challenge in achieving long cycling life. To overcome these issues, we synthesized N-doped graphene quantum dots wrapped with Si nanoparticles (50 nm) compensates the volume expansion and conductivity between neighboring nanoparticles. The introduction of few layers in graphene quantum dots favors in lithium insertion and improved the stability of SEI. This nano-architecture significantly improved the structural stability and conductivity, which could be used as anode material for lithium secondary batteries.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:25

Chair: Tae-Young Kim (GIST)

Preparation of lithium vanadium borate by solid-state method as a cathode for lithium-ion battery

Khoirul Umam, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

The solid-state reaction method has been conducted to prepare of lithium vanadium borate (LVB) as a cathode for lithium-ion battery. Carbon coated LVB has been successfully synthesized to improve the conductivity. Various temperatures are given during the sintering process to reach the highest performance. Prepared LVB has been characterized by X-ray diffraction and ^7Li magic angle spinning NMR spectroscopy. Cyclic voltammetry and long cycle performance have been investigated by charge and discharge instrument with various of C rates.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:30

Chair: Tae-Young Kim (GIST)

Optimal purification method for expression of human melanocortin-4 receptor

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The human transmembrane protein (hTMP) is the type of integral membrane proteins and exists as a signal transduction, intercellular communication, and ion channels, etc. Thus, it has various functions in the biological membrane. In order to demonstrate the function of the transmembrane proteins, the protein should be purified to identify the structure because function is related to structure closely. However, since the transmembrane protein is most composed of hydrophobic amino acids and is surrounded by the lipid, expression and purification of transmembrane protein are not easy. The transmembrane protein, which plays a biologically important role, is associated with the onset of many diseases. If a mutation occurs in human melanocortin-4 receptor (hMC4R), one of the transmembrane proteins, cause eating disorder and obesity. Asparagine-substituted mutants in aspartic acid, the 90th amino acid in the second transmembrane protein (TM2), were found in the patients with early onset obesity. It was thought that the loss of function was caused by structural changes of hMC4R due to the D90N mutation. Therefore, we examined the structural differences between wild-type hMC4R-TM2 (wt-hMC4R-TM2) and mutant hMC4R-TM2 (m-hMC4R-TM2) after expression and purification of two proteins. In the experimental process, SDS was used as a detergent when separating proteins using FPLC to separate them from impurities using hydrophobicity of target proteins. Afterwards, purified high yield target proteins were obtained by using SDS removal method, and the final structure was confirmed by various spectroscopic methods like MS, CD, solution NMR spectroscopy, and solid-state NMR spectroscopy.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:35

Chair: Tae-Young Kim (GIST)

Refractive Index Sensitivity of Localized Surface Plasmon Resonance Inflection Points in Single Gold Nanoparticles with Different Shapes

Hui Bin Jeon, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Plasmonic gold nanoparticles exhibit unique size- and shape-dependent optical properties, which is caused by the localized surface plasmon resonance (LSPR) collective oscillation of conduction electrons in gold with the incident light. In this study, we investigated the medium refractive index (RI)-dependent optical properties and LSPR sensitivity of single gold nanocubes (AuNCs) and gold nanospheres (AuNSs) of similar size (50 nm) under dark-field (DF) microscopy at the single particle level. We found that AuNCs with vertices have higher sensitivity to the medium RI than spherical AuNSs. Furthermore, the LSPR inflection point (IF) at the longer wavelength showed higher RI sensitivity in single particle scattering spectra. Therefore, we provide a deeper insight into the shape-dependent optical properties and RI sensitivity of LSPR IFs at single particle level, which can be beneficial and helpful for their uses in the development of sensitive biosensors.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:40

Chair: Tae-Young Kim (GIST)

Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS

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Lipids are the basic building blocks of cell membrane and are the sources of energy production and the crucial signaling molecules in controlling metabolism through activating or deactivating protein kinases, hormones or related metabolites. With lipid alteration in aging, however, these regulation processes gradually lose their control, and then eventually result in age-related diseases such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Although a number of studies have been conducted to reveal the relationship between age-related diseases and lipids, only few studies have compared lipid changes with aging effect. In this study, lipid profiles in serum, kidney, and heart from C57BL/6 aging mice were examined to understand aging effect solely. Genetically well-controlled and raised 4 and 25-month-old mice which represent young and aged were analyzed by nanoflow ultrahigh pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Above 350 lipid species were identified from each sample group and 163 from serum, 210 from kidney, and 202 from heart were quantified with internal standards of each class. From quantification, most significantly changed (> 1.5 fold and $p < 0.01$) lipid species were found to be down-regulated by aging, but PG and TG species were distinctively up-regulated in heart.

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

Oral Presentation of Young Analytical Chemists I

Room 321, THU 10:45

Chair: Tae-Young Kim (GIST)

A SERS-based microdroplet chip for simultaneous immunoassays of dual prostate cancer markers

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For the fast and accurate detection of prostate cancer markers, a novel surface-enhanced Raman scattering (SERS)-based microfluidic chip was developed for the simultaneous detection of free prostate-specific antigen (f-PSA) and total PSA (t-PSA) markers. In this study, we described a fully automatic droplet-based microfluidic platform for the rapid and sensitive detection of f-PSA and t-PSA. The device was composed of three compartments: mixing and reaction, auto separation, and SERS detections. Sandwich immunoassays for f-PSA and t-PSA biomarkers were performed using sequential microdroplets to avoid tedious washing steps. Raman signals of sequential droplets including supernatant solutions were measured for the quantitative analysis of the PSA markers. The results showed a good linear response for both PSA markers in the range from 0.05 to 100 ng mL⁻¹. The limits of detection were estimated to be below 0.1 ng mL⁻¹ for both the f-PSA and t-PSA. This low LOD level demonstrates that the detection limit of our SERS-based microfluidic immunoassay is much lower than the clinical threshold. Therefore, our proposed method is a very promising clinical tool for the PSA-based screening test of prostate cancer. References 1.R. Gao, Z. Cheng, X. Wang, L. Yu, Z. Guo, G. Zhao, J. Choo, *Biosens. Bioelectron.*, 119, 126 (2018). 2.Z. Cheng, N. Choi, R. Wang, S. Lee, K.C. Moon, S.-Y. Yoon, L. Chen, J. Choo, *ACS Nano*, 11, 4926 (2017). Keywords: SERS, microdroplet device, PSA, multiplex immunoassays

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:00

Chair: Seunghyun Lee (Gachon University)

Prediction of chromatographic elution order using mathematical optimization in QSRR modelling as a means accurate characterization of complex protein mixture

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High-performance liquid chromatography in the reverse-phase separation mode (RP-HPLC) accounts for more than 90 % of separations in modern analytical laboratories. Prediction of liquid chromatography (LC) retention time has become valuable, powerful and routine in method development. While numerous studies have been reported on prediction of retention time, studies on prediction of chromatographic elution order has been very sparse although it is one of the crucial steps in LC retention modelling and prediction. In this work, a first of its kind prediction of elution order is carried out. Elution order prediction is defined as a multi-objective optimization (MOO) problem in quantitative structure-retention relationships (QSRR) modelling with two different objective functions: root mean square error (RMSE) for predicting retention time and sum of ranking difference (SRD) for predicting elution order. For regression modelling, partial least squares (PLS) and artificial neural networks (ANN) are used. Results show that the proposed method as considerably increases computational time but gives more accurate prediction of retention order in case of some columns over a conventional QSRR model. In case of PLS as regression, the proposed method shows mostly incremental improvements of elution order for the Xterra column (tG-20min, T=40 °C) with model error up to 10%. for the same column ANN shows considerable improvement over that of PLS.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:15

Chair: Seunghyun Lee (Gachon University)

Simultaneous Determination of Highly Acidic Glycans in Biotherapeutics using a Combination of PGC-SPE and LC-MS/MS

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Glycosylation of therapeutic glycoproteins affects the pharmacological functions including efficacy, safety, and biological activity of the drug. During the manufacturing process, various media-experimental conditions can lead to alterations in glycosylation. Therefore, overall glycan profiling, including both targeted and untargeted species, should be performed for drug QA/QC. In particular, acidic glycans including sialylated and phosphorylated glycans were directly associated with in vivo functions such as extended serum half-life, protein transfer, and immunogenicity. Despite the biological importance of acidic glycans, their analysis is still highly challenging due to the different physico-chemical properties. Here, we developed an efficient strategy providing high separation selectivity for simultaneous analysis of various acidic glycans using the combination of porous graphitized carbon-solid phase extraction (PGC-SPE) and high resolution LC/MS. For enhanced separation performance, diverse acidic glycans were pre-fractionated according to molecular size and polarity (acidity) using SPE with a PGC cartridge. Subsequent LC-MS and -MS/MS analyses enabled us to obtain glycan compositions, structures, and quantitative information of acidic glycans. We performed glycomic characterization of acidic glycans in a representative therapeutic enzyme, agalsidase-beta, to verify the method. Phosphorylated and sialylated glycans were successfully determined with high selectivity without any ion suppression/interference during LC/MS analysis. We have found high similarities to acid glycans between different batches of therapeutic enzymes. These results show that our method can be applied to assess the equivalence of biological drugs.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:30

Chair: Seunghyun Lee (Gachon University)

Dispersive Liquid-Liquid Microextraction based on Deep Eutectic Solvent for the HPLC-UV Determination of Resveratrol, Oxyresveratrol and Piceatannol from Wine

Jongsung Noh, Seung-Ho Lee, Hyun-Woo Cho¹, Seung Woon Myung*

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Polyphenols are phytochemicals that exist in various plants and are beneficial to human health. These ingredients prevent aging, protect the skin from ultraviolet rays, improve brain health and prevent dementia. Resveratrol, oxyresveratrol and piceatannol in grapes are typical polyphenols, and grape wine also contains these ingredients. In this study, resveratrol, oxyresveratrol and piceatannol in wine were extracted by deep eutectic solvent based dispersive liquid-liquid microextraction (DLLME) and a method for quantification these polyphenols using high performance liquid chromatography - UV/vis spectroscopy was established. Parameters for sample clean up and concentration were optimized and verified. Experiments were carried out to obtain optimal parameters such as the types and volumes of extraction solvent and dispersive solvent, molar ratio of hydrogen bonding donor and hydrogen bonding acceptor, ratio of deep eutectic solvent and water, the pH effect, and the effect of salt. Chromatographic separation with HPLC/UV-vis was performed using the eclipse XDB-C18 (2.1 mm id × 150 mm length, 4.6 μm particle size) column and gradient elution mode using water and acetonitrile. The established method would be applied to wines sold in the market and monitored.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:35

Chair: Seunghyun Lee (Gachon University)

Development of integrated Correlative Light and Electron Microscope

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Light microscopes can obtain color information but do not provide resolution below submicron. The electron microscope can provide much higher resolution information in nanometer scale, but it has the disadvantage that the image is grayscale. As a result of changing the source of the microscope from light to electrons, high resolution was achieved, but the most important visual information, the color, was lost. In order to solve these problems, recently a Correlative Light and Electron Microscope(CLEM) has been developed by integrating a light microscope and an electron microscope, and related researches have been actively conducted. Capability of acquiring color-based information as well as nanometer scale surface information of a sample gives users a new possibility in their research. Previously, samples were observed by a light microscope, and then transferred to an electron microscope. However, in this case, the time and space efficiency is poor, and the sample can be damaged during the transfer of the sample. However, the microscope developed by ourselves has the advantage of reducing the chance of sample damage and observation time because there is no need to move the sample by operating the light microscope and electron microscope simultaneously inside the vacuum. For the identification of defects such as quantum dots and LEDs, a resolution of less than a micrometer(μm) is required, but a light microscope can not show microscopic defects due to the resolution limit. Since the light and the electron beam provide complementary information, it is required to develop a fusion microscope that observes the sample with visible light and enlarges the suspected region using electrons. In this study, we introduce an iCLEM that can present images in real time by integrating light microscope and electron microscope into one system. The light path of the light microscope is positioned inside the optics of the electron microscope so that the coaxial alignment is achieved. This makes it possible to acquire images of fluorescent images and electron microscopes at high magnifications without moving the sample in the vacuum chamber. The iCLEM may

provide researchers with diverse applications in inspection and analysis where a wider resolution spectrum is required in the future.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:40

Chair: Seunghyun Lee (Gachon University)

Evaluation of Fuzzy Rule Building Expert System Tree and Restricted Boltzmann Machine for NIR Spectroscopic Identification of Geographical Origins of Agricultural Products

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Fuzzy rule building expert system tree (FuRES) and Restricted Boltzmann machine (RBM) have been evaluated as a potential method for NIR spectroscopic identification of geographical origins of agricultural samples. FuRES is a tree algorithm with fuzzy expression of classification entropy. FuRES has benefits from simulated annealing and gradient optimization. Restricted Boltzmann machine (RBM) is a restricted form of Boltzmann machines with gradient descent and back-propagation. It can be trained in either supervised or unsupervised ways, depending on the task. In this study, RBM is applied for supervised classification and unsupervised way to extract features. For the evaluation, NIR spectra of imported and domestic agricultural samples (8 different samples: adzuki, angelica root, bellflower root, bracken, carrot, green kernel black bean, kidney bean and perilla seed) were used. For each sample, the discrimination accuracies were acquired using both methods and compared with those using conventional methods such as linear discriminant analysis (LDA) and support vector machine (SVM). The advantages and disadvantages of FuRES and RBM, and their potential in vibrational spectroscopic discriminant analysis will be discussed.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:45

Chair: Seunghyun Lee (Gachon University)

Synthesis of vanadium based polyanion cathode materials for lithium-ion battery

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Lithium-ion batteries are promising energy storage technologies for portable electronic devices such as smart phones, camcorders, and laptops. Lithium vanadium pentoxide has been extensively studied as cathode material in lithium-ion batteries due to its ability for accept lithium ions. However, there is a disadvantage that structural instability occurs when a lot of lithium ions accepted. For this reason, we have replaced borate anion and synthesized carbon-coated lithium vanadium borate which may be expected enhancement of electrochemical properties and structural stability. We expected that the borate anion would lead to increase in structural stability and electric conductivity. The electrochemical properties of lithium vanadium borate were characterized by cyclic voltammetry (CV) measurement for reversibility of lithium extraction/inserting processes.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:50

Chair: Seunghyun Lee (Gachon University)

Analysis of polyglycerophospholipids using isotope-labeled methylation

JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Polyglycerophospholipids (PGPLs) are divided into phospholipids (PLs) containing two glycerols including phosphatidylglycerol (PG), bis(monoacylglycero)phosphate (BMP), hemi BMP, and bis(diacylglycero)phosphate (BDP), and PLs with three glycerols such as cardiolipin (CL), monolysocardiolipin (MLCL), and dilyocardiolipin (DLCL). PGPLs are synthesized from PG and closely related to each other. Since PGPLs have been reported to be associated with neurodegenerative diseases, accurate determination of these lipids is important. Isotope-labeled methylation (ILM) method using (trimethylsilyl)diazomethane (TMSD) can be utilized for relative quantitation of lipids without the addition of internal standard lipids. In addition, many lipids of trace amount could be detected by ILM method with low detection limit. In this study, analysis of PGPLs with ILM method was carried out using nUHPLC-ESI-MS/MS. The collision-induced dissociation (CID) experiments were conducted for the methylated standard PGPLs. The efficiency of methylation for these lipids was found to be > 97% and the degree of methylation was dependent on the number of phosphate groups (1: PG, BMP, Hemi BMP and BDP, 2: CL, MLCL and DLCL). PG and BMP, which are geometrical isomers, and three isomers of BMP can be resolved from each other. A good linear relationship between experimental mixing ratio and calculated peak area of H-/D- methylated lipids were observed. This method was applied to the investigation of PGPLs from a neuronal cell line (SH-SY5Y) which was treated with some drugs, commonly used for the Parkinson's disease model, were quantitatively analyzed.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 09:55

Chair: Seunghyun Lee (Gachon University)

Low-cost plastic devices for drug-resistant pathogen detection in point-of-care setting

Jihyo Park, Seonki Hong*

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World health organization (WHO) warns against 'post-antibiotic' era as a consequence of the rapid emergence of drug-resistant pathogens, so called superbugs, that are not treated by most of antibiotics. Advanced diagnostic techniques allow clinicians to prevent inappropriate prescribing and overuse of antibiotics which may delay the emergence of life-threatening pathogens. In this study, we aim to develop a low-cost plastic device for rapid and accurate pathogen detection. We applied a nature-inspired material-independent biosilicification process on the surface of plastics that is difficult to be functionalized by conventional surface chemistry due to intrinsic hydrophobicity and lack of functional groups for bioconjugation. By this approach, the surface of polycarbonate and polypropylene-based plastic devices with micro-pillar structure were successfully decorated by silica so that we could selectively enrich bacterial RNA from whole lysate on the surface of devices. Surface-enriched RNA was further detected by on-chip colorimetric loop-mediated isothermal amplification (LAMP) within 30 minutes.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:00

Chair: Seunghyun Lee (Gachon University)

The Effect of Electrophilicity of Thiol Molecules in Chemical Interface Damping of Single Triangular Gold Nanoplates

Junho Lee, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Plasmonic nanoparticles have been extensively studied for various applications such as photocatalyst, biosensor, orientation probe, photothermal cancer therapy etc. This is because they exhibit unique size and shape dependent optical properties resulted from the localized surface plasmon resonance (LSPR) effect. The LSPR is vibration of free electrons in the conduction band induced by interaction with an electromagnetic field. Recently, two-dimensional (2D) triangular gold nanoplates (AuNPs) are of great interest in many applications such as nanocatalysis and biosensors due to their characteristic LSPR property caused by triangular shape. However, chemical interface damping in single AuNPs at the single particle level has not yet been studied so far. In this study, we characterized the optical properties of single AuNPs and thiolate effect under dark-field (DF) microscopy. The LSPR damping was observed for single thiol-capped AuNPs due to chemical interface damping effect on their surface under single particle scattering spectroscopy. Furthermore, thiol molecules with strong electron withdrawing group (EWG) was compared to strong electron donating group (EDG) on chemical interface damping in single AuNPs. Therefore, we found the potential use of single AuNPs as plasmonic biosensors using this chemical interface damping.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:05

Chair: Seunghyun Lee (Gachon University)

Multi-channel Microchip Electrophoresis for Rapid Screening of Glutathione S-transferase Polymorphism Genotyping

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A voltage programming (VP)-based microchip electrophoresis (ME) method was developed to detect specific sizes of DNA fragments. The optimum condition was deliberated on a single-channel microchip and was then applied to a multi-channel microchip for simultaneous high-throughput detection. Glutathione S-transferase (GST) polymorphism genes (M1/M1 = 215 bp/215 bp, M1/T1 = 215 bp/480 bp, and T1/T1 = 480 bp/480 bp) extracted from human blood were amplified by polymerase chain reaction and were introduced into the multi-channel microchip. Target DNA molecules amplified by only 10 PCR cycles could be detected by the VP-based multi-channel ME, but not by slab gel electrophoresis. Besides, the migration time for ME was less than 15 s which was 700 times faster than SGE. Furthermore, internal control (312 bp) was added for further identification of target DNA. The presented modality was demonstrated to be effective and rapid for highly sensitive and high-throughput screening of GST genes.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:10

Chair: Dukjin Kang (KRISS)

Profiling of oxidized phospholipids in exosome and subcellular species of cells under oxidative stress by flow field-flow fractionation and nUHPLC-ESI-MS/MS

JoonSeon Yang, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Oxidative stress occurs when production of reactive oxygen species (ROS), which include oxygen derived radical species such as superoxide anion (O_2^-) and hydroxyl radical ($\cdot OH$) as well as hydrogen peroxide (H_2O_2), exceeds removal capacity of antioxidants. Moderate concentration of ROS is related to some beneficial physiological roles (e.g. signaling, host defense), but high levels of ROS not only induces cellular impairments by altering DNA, RNA, proteins, and lipids but also involves with a number of diseases like cardiovascular disease (CVD) or cancer. Exosomes are nano-sized extracellular vesicles secreted from cells. It has been reported that exosome transports some protective RNA against oxidative stress or transfers stress signals to recipient cells, when oxidative stress is given to cells. However, physiological roles or changes of lipids in exosome during oxidative stress conditions have not yet been studied. In this study, oxidative stress was induced to human embryonic kidney cell 293 (HEK293) by treating with H_2O_2 for 72 hours. Exosome and cellular organelles from control and oxidatively stressed conditions were size-sorted by flow field-flow fractionation first. Then, changes in lipid profiles in cell and exosome was conducted by nUHPLC-ESI-MS/MS.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:15

Chair: Dukjin Kang (KRISS)

Effects of *Ecklonia cava* extract intake on endogenous and exogenous metabolites in human urine

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Ecklonia cava is a sort of brown algae native to Korea and Japan, containing unique polyphenols referred to as phlorotannins. Recently, several studies have been examined the effect of phlorotannins, which reduces body fat and improves cardiovascular function. However, there are few metabolic studies relevant to those effects in human model. In this study, we performed a comprehensive metabolomics analysis of urine from males and females with a BMI over 25kg/m² and under 30kg/m² using ultra-performance liquid chromatography quadruple time-of-flight mass spectrometry (UPLC-Q-TOF-MS) to investigate effects of *Ecklonia cava* extract (Seapolynol) intake on the exogenous and endogenous metabolites. Statistical analysis were performed with correlation analysis and Hierarchical clustering analysis. We found that several endogenous and exogenous metabolites were significantly associated with Seapolynol intake, such as sulfonic acid, organic acid, xanthine and flavonoid glycoside. Especially, the levels of methyl xanthine and methyl uric acid were increased, whereas flavonoid glycoside was decreased in Seapolynol group. This study demonstrates that UPLC / MS based urine metabolic approach can be used to investigate the metabolic effects of Seapolynol intake and provide the insight for metabolism.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:20

Chair: Dukjin Kang (KRISS)

Comparative Analysis of Lectin based Glycoproteomics and Triglyceride and Glucose (TyG) Index between Elderly Yoga Groups

Miseon Jeong, Jinwook Lee¹, Wonryeon Cho*

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We had already investigated the efficacy of elderly yoga by identifying and comparing the glycoproteins in human plasma. This study focused on comparing the efficacy of yoga with the change of Triglyceride and Glucose (TyG) Index from Advanced level group and Beginner level group. The TyG Index can predict diabetes with simple calculation. The glycoproteins from the yoga participants' plasma are affinity selected using self-packed *Lycopersicon esculentum* lectin (LEL) columns. After that, peptides from affinity selected proteins were deglycosylated with PNGase F and identified with nLC-MS/MS. The results show that the number of plasma glycoproteins in Advanced level group is less than that in Beginner's group, demonstrating an inverse correlation between number of plasma glycoproteins and yoga experience. Additionally, the decrease of TyG Index in Advanced level group is higher than Beginner level group, which is similar to the tendency of glycoprotein change between elderly healthy yoga groups.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:25

Chair: Dukjin Kang (KRISS)

Support Effect of Plasmonic Nanoparticles on Carbon Nanotubes at Single-molecule Level

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Supported catalysts were synthesized with gold nanoparticles deposited on the outer surface (Au/CNTs-out) and inner surface (Au/CNTs-in) of CNTs by wet chemistry method. Single-molecule nanocatalysis measurements were carried out using a lab-built prism-type total internal reflection fluorescence microscope (TIRFM) by detecting the fluorescence from the reduction reaction catalyzed over Au/CNTs-out and Au/CNTs-in. The results indicated the support effect of CNTs in both product formation process and product dissociation process. For the product formation process, Au/CNTs-out showed higher catalytic activity than Au/CNTs-in because gold nanoparticles on the exterior of CNTs have relatively enriched electrons compared to those on the interior walls. For the product dissociation process, Au/CNTs-out exhibited the faster product molecules dissociation rate than Au/CNTs-in. Moreover, same dissociation pathway was observed. Product molecules on both Au/CNTs-out and Au/CNTs-in preferred the reactant-assisted dissociation pathway. Our research advances the traditional single-molecule method to provide insights into the supported catalysts.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:30

Chair: Dukjin Kang (KRISS)

Design of truncated-IK protein's derivatives that alleviate inflammation

Hyunjun Jang, Ji Sun Kim , Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Rheumatoid arthritis is a chronic inflammatory disease. In Rheumatoid arthritis, activated immune cells attack the synovial membrane, cartilage and bone of the joints. So, the synovial membrane is abnormally proliferated and the bones and joints are destroyed. Although there are many causes for the disease, it is known that self-antigen recognition through abnormal MHC class II-expressing B cells excessively produces antibodies. Recent studies have shown that inhibitor K562 leukemic cell has been isolated and purified from the conditioned culture medium. This truncated IK (tIK) downregulates MHC class II on activation in inflammatory diseases. In our study, we examined the phosphorylation pattern of protein cell signaling by isolating macrophages from transgenic mice transplanted with the tIK nucleotide sequence, and found that tIK protein had the same effect as the anti-inflammatory cytokine IL-10. Therefore, we focused on the process of finding derivatives that are shorter and better anti-inflammatory than the previously reported tIK protein. We predicted the possible structure of tIK based on IL-10 through sequence homology modeling and could derive an epitope associated with anti-inflammatory activity. Based on these results, we proposed 4 anti-inflammatory peptide candidates and identified the anti-inflammatory activity through the TH17 cell differentiation test. Among them, the 18-mer peptide with anti-inflammatory activity was named tIK-YK4 and the short derivatives 9-mer and 14-mer peptides were also designed. Currently, we have successfully performed overexpression using *E. coli* and are optimizing the purification process. We are confirming peptide candidates using various techniques such as PAGE, CD, MASS.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:35

Chair: Dukjin Kang (KRISS)

Preparation of borovanadate system as cathode material for lithium ion batteries

Chaewon Moon, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Lithium-ion batteries are the most important energy storage system for wide applications in electronic portable devices and hybrid electric vehicles. Lithium ion battery consists of four major components such as anode, cathode, electrolyte, and the separator. During the charging process, lithium ions are released from the cathode and transferred to anode through the electrolyte, and this process is reverse during the discharge process. As a cathode material of Li-ion battery, typical vanadium-containing phosphate, $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (LVP), has a high theoretical specific capacity of 197 mAh g^{-1} for the multiple valence state of the vanadium element. In addition, vanadium-contained phosphate has excellent thermal stability and contributing to good cycle stability during the charge and discharge processes. In this study, a lithium borovanadate system, which is a vanadium-contained borate, was prepared via sol-gel method. And its electrochemical properties of samples were investigated. The electrochemical properties of samples were investigated through lithium extraction/inserting processes using galvanostatic charge/discharge and cyclic voltammetry (CV) measurements so as to investigate for Li^+ ion transfer between the active electrode materials.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:40

Chair: Dukjin Kang (KRISS)

A study on the determination of inorganic arsenic by solid phase extraction and laser ablation inductively coupled plasma mass spectrometry

Seon Hwa Lee, Sang-Ho Nam*

Department of Chemistry, Mokpo National University, Korea

The toxicity and chemical properties of arsenic depend on the concentration and chemical structure present in the natural environment. Inorganic arsenic is more toxic than organic arsenic, thus the accurate determination of inorganic arsenic in various samples is needed. IC-ICP-MS (Ion Chromatography-Inductively Coupled Plasma-Mass Spectrometry) is the current method for quantitative and qualitative determination of arsenic. However, the method has disadvantage of expensive and complex instrument, and elaborate sample preparation. In this study, inorganic arsenic species were separated using a membrane filter disk in the SPE (Solid Phase Extraction) method, then determined by LIBS (Laser Induced Breakdown Spectroscopy) and LA-ICP-MS (Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry). The detection limit of inorganic arsenic is 10 mg/kg by the SPE membrane filter with LIBS. The detection limit of inorganic arsenic was 1.0 $\mu\text{g}/\text{kg}$ by LA-ICP-MS. The pH value of the sample was adjusted to 4 using ammonium hydroxide and phosphoric acid for the efficient separation of inorganic arsenic species. The linear dynamic range was from 1 to 1000 $\mu\text{g}/\text{kg}$ by LA-ICP-MS, and the correlation coefficient was 0.9997. A new method using solid phase extraction and LA-ICP-MS was a accurate and sensitive method for quantitative analysis of inorganic arsenic in a sample.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:45

Chair: Dukjin Kang (KRISS)

Analysis of characteristic serum lipids of post-hepatectomy liver failure from partially hepatectomized swine using nanoflow UHPLC-ESI-MS/MS

HaeA Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Since liver possesses the big capacity to regenerate, hepatectomy is a common treatment for the disease like hepatocellular carcinoma. However, liver resections are complex operations and have a risk of complication. Especially, post-hepatectomy liver failure (PHLF) which is a liver failure after operation is one of the most serious complications and a big part of the reason of death. Liver has an important role in lipid metabolism. Therefore if liver doesn't function properly, the homeostasis of lipids might be failed. In this study, the changes of lipid profiles of swine serums were observed depending on rate of hepatectomy and time after operation using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS) to give more accurate insight into PHLF. The swines were divided into fake operation group (sham, n=6), 70% partial hepatectomy group (70% PHx, n=7), and 90% partial hepatectomy group (90% PHx, n=7). The serums were collected before operation, and 14 hours, 30 hours, and 48 hours after operation from each groups. The extracted lipids were structurally identified based on collision-induced dissociation (CID) experiments and individual serums were quantitatively analyzed through selective reaction monitoring (SRM) mode. The identified lipids were 142 phospholipids, 23 sphingolipids, and 240 glycerolipids.

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

Oral Presentation of Young Analytical Chemists II

Room 321, FRI 10:50

Chair: Dukjin Kang (KRISS)

Plasmonic sensing of biotin-BSA proteins by chemical interface damping of single gold nanorods.

SeongWoo Moon, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Chemical interface damping (CID) is one of the main decay processes that result in the broadening of the homogeneous localized surface plasmon resonance (LSPR) linewidth in plasmonic gold nanoparticles. However, it is the most poorly understood damping mechanism in gold nanoparticles. Herein, to better understand CID, we performed scanning electron microscopy (SEM) correlated dark-field (DF) scattering studies of single gold nanorods (AuNRs). First, we examined size-dependent broadening of the homogeneous LSPR linewidth in single AuNRs with three different aspect ratios (ARs) at a fixed diameter of 25 nm. The LSPR linewidth increased with decreasing the AR of single AuNRs because of the reduced average distance of hot electrons to the surface. Second, we examined the effect of adsorbate thiol molecules on the homogeneous LSPR linewidth in single AuNRs. The LSPR linewidth was broadened with increasing the carbon chain length of 1-alkanethiol. Third, we investigated the effect of refractive index variation of the surrounding medium on the LSPR linewidth in single AuNRs of three different sizes. The LSPR linewidth remained almost constant while increasing the dielectric constant of the medium. Last, we confirmed that CID-based biosensors can be used to detect real biological molecules such as bovine serum albumin (BSA) conjugated with biotin.

Award Lecture in Division : **LIFE.O-6**

Oral Presentation of Young Biological Chemists

Room 314, THU 10:30

Chair: Kwang Pyo Kim (Kyung Hee University)

Cell-based phenomics study using chemical probe

Jun-Seok Lee

*Molecular Recognition Research Center / Korea Institute of Science and Technology, Bio-Med Division,
Korea*

In 1665, Robert Hooke peered down his microscope at cork and reported the empty spaces contained by walls that he dubbed "Cell". As the minimum building block of all life, cells constitute a living organism, and individual cell expresses unique transcriptome that regulates the function & fate of the cell. With the recent dramatic developments of single-cell analysis techniques, we are getting to understand the diversity of cells, but the task of cataloging the 37.2 trillion cells of the human body is still in an early stage. In this seminar, I will talk about how a chemical probe plays a role as the phenomics tool using differential sensing approach, and discuss the perspective of at the cell atlas study.

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

Oral Presentation of Young Biological Chemists

Room 314, THU 09:00

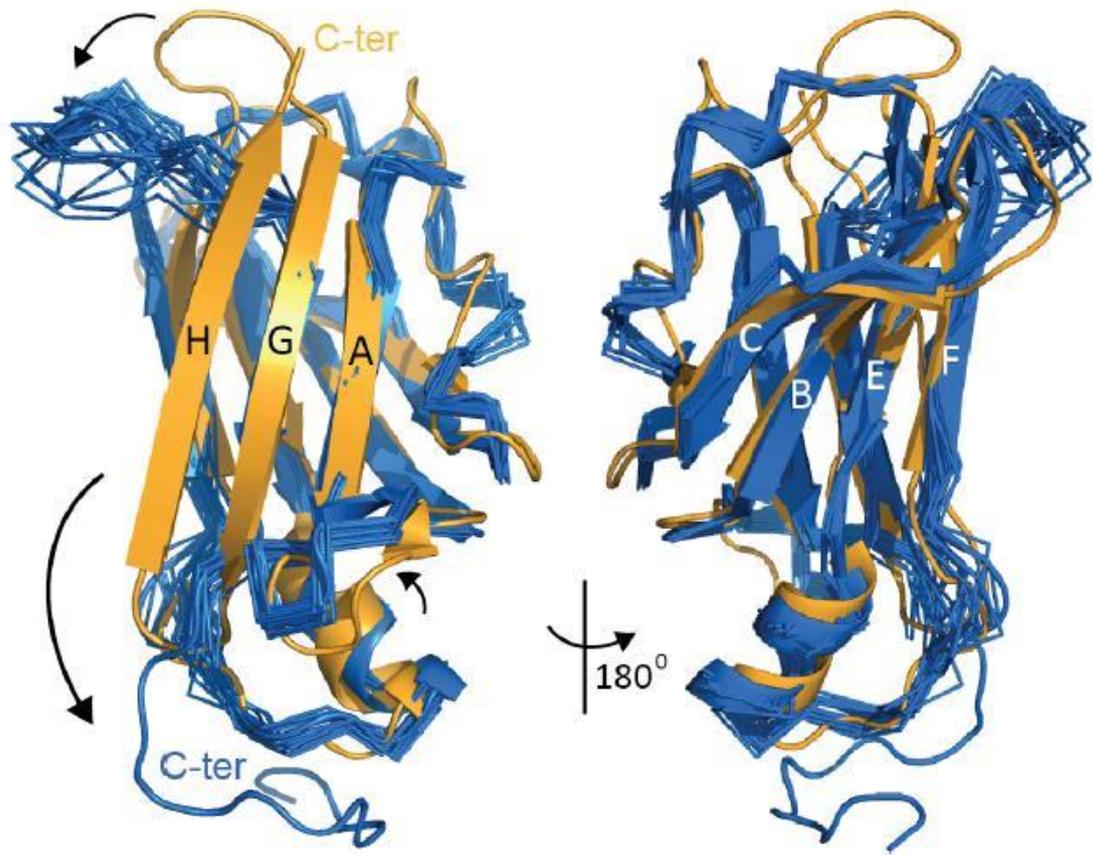
Chair: Young-Sam Lee (DGIST)

The solution structure of transthyretin in its monomeric aggregation-prone state

Jin Hae Kim

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

Transthyretin (TTR), in its native tetrameric state, is an essential transporter of thyroxine and holo-retinol binding protein for human. However, its dissociation into the mis-folded monomer facilitates abnormal aggregation of TTR, causing deposition of TTR aggregates typically in the peripheral nervous system or in the heart. Although understandings to this TTR-aggregation mechanism have succeeded to develop effective therapeutics stabilizing the tetrameric state of TTR, it is still elusive which structural transition is indeed responsible for its aggregation. Here, we determined with nuclear magnetic resonance (NMR) spectroscopy the three-dimensional structures of the two TTR variants: amyloidogenic monomeric TTR and its protective (less amyloidogenic) variant, T119M. Distinctive to the native tetrameric state, the misfolded monomer of TTR presented structural features in which the C-terminal beta-strand is released and the neighboring loops are perturbed (refer the attached figure). On the other hand, introduction of T119M mutation caused non-native rearrangement of the beta-strand structure; it appears that this structural transition damped conformational fluctuations of the C-terminal beta-strand, which is known to be important for TTR aggregation.



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

Oral Presentation of Young Biological Chemists

Room 314, THU 09:20

Chair: Young-Sam Lee (DGIST)

Plausible way for abiotic production of ribonucleosides

Inho Nam

Chemistry and Bio-Environmental Sciences, Seoul Women's University, Korea

The feasibility of the abiotic fabrication of ribonucleosides which are the building blocks of ribonucleic acid (RNA) has been questionable because a condensation reaction between ribose and nucleobases is thermodynamically unfavorable in bulk environment. Here, I describe an abiotic synthetic path for ribonucleosides, both purine and pyrimidine ribonucleosides in water microdroplets, following a salvage reaction pathway in cells. The abiotic reaction path includes a condensation reaction between ribose and phosphate to give ribose 1-phosphate and an exchange reaction between nucleobase and phosphate in the ribose 1-phosphate. The reaction steps were forced by water microdroplets that changes the thermodynamic property of condensation reaction and accelerated by divalent magnesium ion, Mg^{2+} , as a catalyst. In the bulk environment, the condensation reaction for giving ribose 1-phosphate has the positive value of Gibb's free energy change (ΔG). However, ΔG changes to the negative value in microdroplets, which makes the abiotic salvage pathway spontaneous. Consequently, both types of ribonucleosides, purine and pyrimidine ribonucleosides, could have arisen through the same chemical environment, which means that simultaneous production of random ribonucleosides might be possible for generating chains of RNA in microdroplets.

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

Oral Presentation of Young Biological Chemists

Room 314, THU 09:40

Chair: Young-Sam Lee (DGIST)

Single Molecule Approach for Cell Biology; Control of Notch and Cadherin Signaling at Single Cell Level

Daeha Seo

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

Tools capable of imaging and perturbing mechanical signaling pathways with fine spatiotemporal resolution have been elusive despite their importance in diverse cellular processes. The challenge in developing a mechanogenetic (i.e. genetically encoded mechanical perturbations) toolkit stems from the fact that many mechanically-activated processes are localized in space and time, yet additionally require quantitative mechanical loading to become activated. To address this unmet need, we synthesized magnetoplasmonic nanoparticles that can image, localize, and mechanically load targeted proteins with high spatiotemporal resolution. We demonstrate their utility as a quantitative perturbation system by investigating the cell surface activation of Notch and E-cadherin receptors. By measuring cellular responses to various spatial, chemical, temporal, and mechanical inputs at the single molecule and single cell level, we reveal how spatial segregation and mechanical force cooperate to direct receptor activation dynamics. This generalizable technique can be used to control and understand diverse mechanosensitive processes in cell signaling.

General References

- (1) Daeha Seo, Kaden M. Southard, Ji-wook Kim, Hyunjung Lee, Justin Farlow, Jung-uk Lee, David Litt, Thomas Haas, Jinwoo Cheon, A. Paul Alivisatos, Zev J. Gartner, Young-wook Jun “A Mechanogenetic Toolkit for Interrogating Cell Signaling in Space and Time” *Cell*, **2016**, 165, 1507.
- (2) Ji-wook Kim, Daeha Seo, Jung-uk Lee, Kaden M. Southard, Yongjun Lim, Zev J. Gartner, Young-wook Jun, Jinwoo Cheon “Single cell mechanogenetics using monovalent magnetoplasmonic nanoparticles” *Nature Protocol*, **2017**, 12, 1871

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

Oral Presentation of Young Biological Chemists

Room 314, THU 10:00

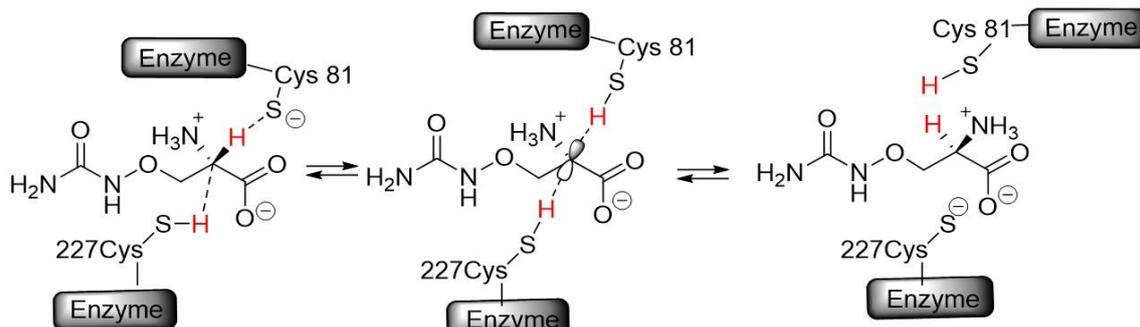
Chair: Young-Sam Lee (DGIST)

Mechanistic studies of O-ureidoserine racemase

Yeong-Chan Ahn, John Vederas*

Department of Chemistry, University of Alberta, Canada

O-ureidoserine racemase (DcsC) is a PLP-independent racemase involved in the biosynthesis of the important antibiotic D-cycloserine. Our goal is to elucidate the mechanism of this unusual epimerization by means of crystallization of the enzyme with a known optically pure inhibitor. Alternatively, the mechanistic information can be achieved by crystallization of the racemic inhibitor with site-specifically mutated DcsC variants. This approach has been shown successfully in proving the proposed epimerization mechanism for the highly homologous diaminopimelate epimerase. With a crystal structure in hand we will be able to visualize the 3D geometry of the active site revealing how DcsC is able to significantly decrease the pKa of the substrate thus enabling the proton abstraction under physiological conditions.



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

Oral Presentation of Young Biological Chemists

Room 314, THU 10:15

Chair: Young-Sam Lee (DGIST)

Target specificity of the CRISPR-Cas9 nuclease regulated by the REC2 domain via structural rearrangement of DNA

Keewon Sung, Jinho Park, Nam Ki Lee, Seong Keun Kim*

Department of Chemistry, Seoul National University, Korea

The RNA-guided CRISPR-Cas9 nuclease cleaves DNA targets using recognition by base-pairing between the RNA and DNA sequences. Originating from an adaptive immune system in prokaryotes, CRISPR-Cas9 has been widely studied for genome engineering applications, but the mechanistic basis of its target specificity still remains to be elucidated to understand and minimize off-target DNA cleavage. In this work, using single-molecule FRET and REC2-mutational analyses, we show that a non-nucleolytic domain within the Cas9 nuclease called REC2 plays a crucial role in enhanced off-target discrimination. Specifically, we find that the REC2 domain regulates structural rearrangement of the non-target strand of DNA for cleavage reaction with the help of positively-charged amino acids on its surface, by inducing a non-cleavable conformation particularly for off-target sequences. This result provides molecular insights for the target-specific activation of the Cas9 nuclease and thereby for rational design of engineered Cas9 toward highly-specific genome editing.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 09:00

Chair: Eun Jin Cho (Chung-Ang University)

Enantioselective Protonation/Nucleophilic Addition and Strecker Reaction Catalyzed by Chiral Oxazaborolidinium Ion

Ki-Tae Kang, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

A new chiral Brønsted acid derived from carboxylic acid and a chiral oxazaborolidinium ion (COBI), as an activator, is introduced. This acid was successfully applied as a catalyst for the highly enantioselective protonation/nucleophilic addition of diazoesters with carboxylic acids. Meanwhile, In the presence of a catalytic amount of COBI, aldimine reacted with trimethylsilyl cyanide (TMSCN) to afford α -aminonitriles in excellent yields and enantioselectivities. The three-component asymmetric process studied here significantly improves upon the original Strecker reaction, and has advantages over previous reactions using unstable imines. High levels of enantioselectivities in the synthesis of α -aminonitrile derivatives with wide substrate generality were obtained via these reactions. The reaction proceeded in good yields (up to 98%) with excellent enantioselectivities (up to 99% ee).

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 09:15

Chair: Eun Jin Cho (Chung-Ang University)

Chemo- and Stereoselective Allylboration of Aldehydes and Cyclic Aldimines with Allylic-gem-diboronate Ester

Jinyoung Park, Yeosan Lee, Seung Hwan Cho*

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

The preparation of new types of organoboron compounds is especially important owing to their stability and ability to undergo a wide range of organic transformations. In recent years, gem-diborylalkanes have emerged as attractive synthetic intermediates for synthesizing organoborons via transition-metal-catalyzed or transition-metal-free chemo- and stereoselective transformations with suitable electrophiles. Although considerable advances have been made in recent years, most of the methods developed employed alkyl-substituted gem-diboron reagents, the use of which necessitates strong base (MOH or MO-t-Bu, M= Li, Na, K) to activate one of the pinacolato boron (Bpin) units of the gem-diborylalkane chemoselectively through the formation of an α -boryl alkyl metal species or α -borylcarbanion. In this presentation, we report a highly chemo- and stereo selective crotylation of aldehydes and cyclic aldimines with allylic-gem diboronate ester as a new type of organoboron reagent. The allylic-gem-diboronate ester undergoes the crotylation with aldehydes and cyclic aldimines in excellent stereoselectivity, forming anti-5,6-disubstituted oxaborinin-2-ols or (E)- δ -boryl-anti-homoallylic amines in high efficiency. The reaction shows a wide range of substrate scope and excellent functional group tolerance. The synthetic applications of the obtained products, including stereospecific C-C, C-O, and C-Cl bond formation, are also demonstrated.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 09:30

Chair: Eun Jin Cho (Chung-Ang University)

Pd(II)-Catalyzed Regioselective Formation of 1-Hydroxycarbazoles

Youngho Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

Recently, we developed a Pd-catalyzed regioselective cyclization reaction of N-Ts-2-amino-3'-hydroxylbiaryls under mild aerobic conditions to afford 1-hydroxycarbazoles. Dual directing group-assisted C-H activation at the sterically more hindered C2'-position of 2-amino-3'-hydroxylbiaryls appears to occur. Moreover, complicated natural products were successfully synthesized, demonstrating the synthetic utility of this method.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 09:45

Chair: Eun Jin Cho (Chung-Ang University)

Synthesis of Chiral [1,4]-diazocines : Enantioselective Rhodium(II)-catalyzed [5+3] Cycloaddition

Ju Young Lee, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Korea

Eight-membered heterocycles are one of the most significant classes of compounds as it has been found in as key structural motif in a large number of biologically important natural products and pharmaceuticals. Among the established approaches including most popular ring-closing metathesis, Heck or other cross-coupling reactions for the synthesis of such medium-ring heterocycles the higher-order cycloaddition strategy is believed to be hard as it associated with unfavourable enthalpic and entropic parameters. As a consequence, the number of reports describing [5+3] cycloaddition to form eight-membered heterocycles are limited. Recently, our group disclosed a novel intermolecular rhodium(II)-catalyzed [5+3] cycloaddition between pyridinium zwitterions as 1,5-dipole equivalents and enol diazoacetates for the efficient formation of eight-membered heterocycles. Also, we have investigated the detail mechanistic insight of this reaction based on DFT study. Based on our previous results, we developed the asymmetric version of this interesting methodology using a chiral Rh(II)-catalyst and tuning the reaction condition. Despite this initial success, we were unable to apply this protocol as general basis. After extensive screening of the reaction conditions, we envisioned that some structural tuning is required for both the zwitterionic species and the diazo-substrate. In this symposium we will discuss our successful approach towards asymmetric [5+3]-cycloaddition between quinoline-based 1,5-dipole with vinyl diazoacetate partners.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 10:00

Chair: Eun Jin Cho (Chung-Ang University)

The Development of New Nano-Photosensitizer and Overcoming Limits of Photodynamic Therapy

Nahyun Kwon, Juyoung Yoon*

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

Photodynamic therapy (PDT) with its noninvasive characteristic is a promising treatment for cancer. When light activates the photosensitizer, the excited state energy is transferred to the bottom molecular oxygen to produce singlet oxygen, which has high cytotoxicity to the biological tissue. Unfortunately, solubility and tumor targeting of conventional photosensitizers are still unsatisfactory. Patients need to avoid exposing themselves to sunlight and room light during long periods (typically 4-6 weeks) after PDT treatment. Otherwise, "always on" PS causes a harmful photosensitization effect to the skin, eyes and other normal tissues. In addition, the hypoxic environment of tumor tissue seriously inhibits the PDT process that works through oxygen-dependent mechanisms. Recent studies have shown that nano-structured photosensitizer assemblies or nano-delivery systems are useful in overcoming this problem. Nano-photosensitizers can accumulate in tumor tissue due to improved permeability and retention (EPR) effects. Inspired by the well-known prodrug concept and the successful use of concomitant drugs in clinical medicine, we recently developed several approaches to fabricating new nano-photosensitizers and carried out the evaluation of tumor imaging and photodynamic activity.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 10:15

Chair: Eun Jin Cho (Chung-Ang University)

Molecularly Controlled Stark Effect Induces Significant Rectification in Polycyclic Aromatic Hydrocarbon-terminated n-Alkanethiolates

Soojin Cho, Gyu Don Kong, Sohyun Park, Seo Eun Byeon, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Understanding the structure-electric field relationship is a significant challenge in molecular and organic electronics. In this presentation, we will show that reliable and reproducible molecular diode can be achieved through the control of conjugation length in polycyclic aromatic hydrocarbon-terminated n-alkanethiolate (denoted as SC₁₁PAH), incorporated into liquid metal-based large-area tunnel junctions in the form of self-assembled monolayer. By taking advantage of structural simplicity and tunability of SC₁₁PAH and high-yielding feature of the junction technique, we demonstrate the increase in conjugation length of the PAH terminal group leads to significant rectification ratio up to $\sim 1.7 \times 10^2$ at ± 740 mV. Further study suggests that the Stark shift of molecular energy resonance of PAH breaks the symmetry of energy topography across the junction and induces rectification in a temperature-independent charge transport regime.

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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 10:30

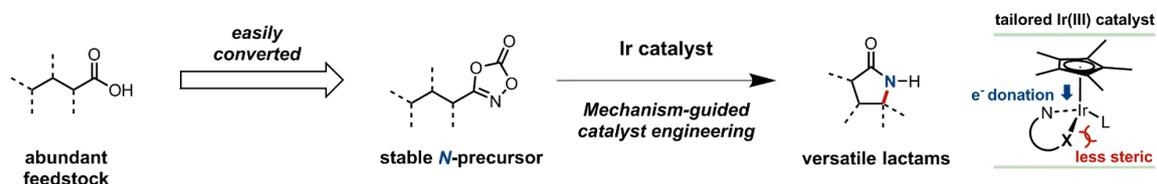
Chair: Eun Jin Cho (Chung-Ang University)

Selective Formation of γ -Lactams via C–H Amidation Enabled by Tailored Iridium Catalysts

Seung Youn Hong, Sukbok Chang*

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

The direct amidation of C–H bonds to obtain nitrogen-containing heterocycles is a highly desirable reaction, because it will open the door to many new applications in chemical synthesis. Although tremendous progress has been made, our current ability to prepare heterocycles via such direct C–H functionalization is limited. Here we present a novel methodology that employs Ir-based catalysts and dioxazolone substrates to access short-lived Ir-nitrenoid complexes, which are key intermediates in the efficient construction of γ -lactams through direct C–H bond amidation. Stoichiometric studies with robust carbonylnitrene precursor, 1,4,2-dioxazol-5-ones, suggest that the insertion of C–H into metal-nitrenoid moiety is possible and mechanistic clues from the initial proof-of-concept studies further enabled the design of efficient and versatile catalysts that allows for the straightforward amidations of various sp^3 - and sp^2 C–H bonds with exceptional selectivity leading to lactam products. The power of this new method is demonstrated in the successful late-stage functionalization of bio-active molecules with amino acid derivatives to produce molecules that are highly sought after for pharmaceutical and other applications in synthesis.



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

Oral Presentations for Young Scholars in Organic Division

Room 325A+B, THU 10:45

Chair: Eun Jin Cho (Chung-Ang University)

A Modular Synthesis of 4-Aminoquinolines and [1,3] N-to-C Rearrangement to Quinolin-4-ylmethanesulfonamides

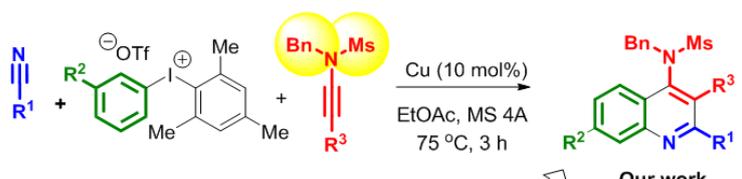
Kyung hwan Oh, Jin Gyeong Kim, Jin Kyoon Park*

Department of Chemistry, Pusan National University, Korea

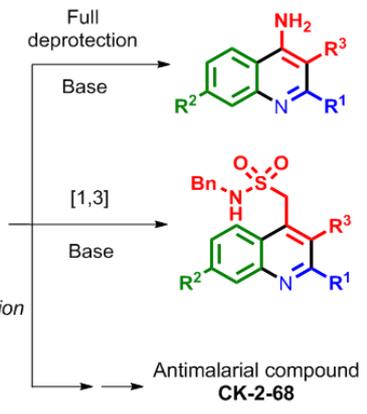
In order to achieve atom economy, efficiency, diversity, and step economy, tandem cyclization could be an efficient strategy for the systematic development of heterocycles in multi-component reactions (MCRs). In this regard, we were interested in the [2+2+2] cycloaddition reaction for the synthesis of 4-aminoquinoline. Herein, we developed copper-catalyzed regiocontrolled three-component reaction allowing systematic functionalization of 4-aminoquinoline using nitrile, iodonium salt and N-benzyl-N-mesylynamide. Furthermore, we explored base-promoted full deprotection of 4-aminoquinolines with potassium butoxide (KO^tBu) and 1,3-rearrangement of 4-aminoquinoline with lithium bis(trimethylsilyl)amide (LHMDS) to provide quinolin-4-ylmethanesulfonamides. Finally, active antimalarial compound CK-2-68^[1] was successfully prepared by our synthetic method.

References

- [1] Pidathala, C.; Amewu, R.; Pacorel, B.; Nixon, G. L.; Gibbons, P.; Hong, W. D.; Leung, S. C.; Berry, N. G.; Sharma, R.; Stocks, P. A.; Srivastava, A.; Shone, A. E.; Charoensutthivarakul, S.; Taylor, L.; Berger, O.; Mbekeani, A.; Hill, A.; Fisher, N. E.; Warman, A. J.; Biagini, G. A.; Ward, S. A.; O'Neill, P. M. J. *Med. Chem.* 2012, 55, 1831 [2] Oh, K. H.; Kim, J. G.; Park, J. K. *Org. Lett.*, 2017, 19, 3994



Regioselective regioisomer formation at challenging C7 position from meta-substituted phenyliodonium salt



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

Oral Presentation of Young Material Chemists

Room 322, THU 09:00

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Light-induced electrical switch via photo-responsive nanocomposite film

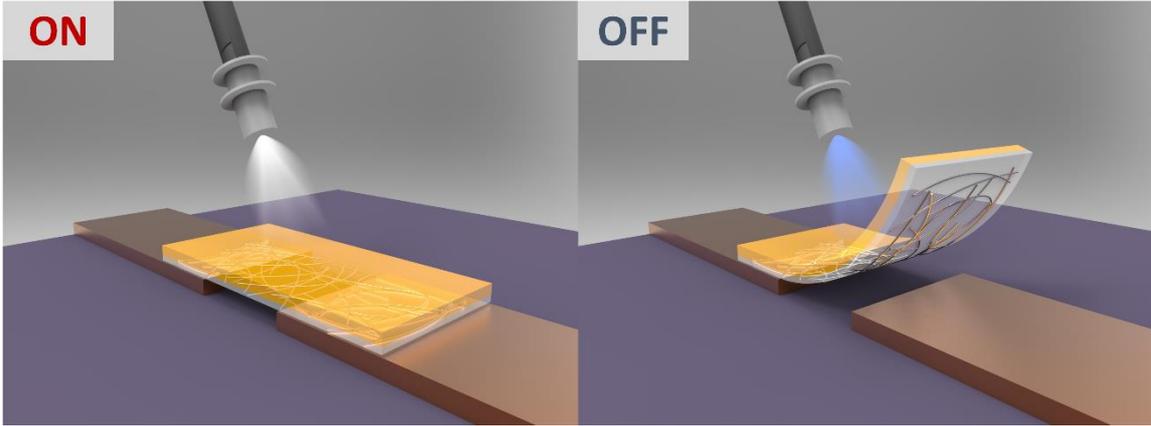
Wonsik Lee, Dongjun Kim¹, Geonho Kim, Ikyon Kim^{2,*}, Jiwon Kim*

School of Integrated Technology, Yonsei University, Korea

¹*School of integrated technology, Yonsei University, Korea*

²*Department of Pharmacy, Yonsei University, Korea*

Photo-responsive nanomaterials have attracted a lot of attention since they allow a remote control with a non-invasive stimulus—light. Owing to this property, it has been applied to next-generation electrical devices, which are desired to be flexible and transparent for a wider range of applications. Herein, we developed a flexible, transparent and conductive film which can change its shape *via* light of specific wavelength to control the electrical conductivity between electrodes. The film is composed of three layers: azobenzene incorporated poly(dimethylsiloxane), AzoPDMS; silk fibroin; and silver nanowires, AgNWs. When azobenzene within the polymer changes its molecular arrangement upon irradiation, the difference in volume changes of AzoPDMS and silk fibroin layer results in the film to bend. Since a silk fibroin layer folds inward upon irradiation, AgNWs are coated onto the silk fibroin layer to be selectively in contact with the electrodes. This photo-responsive nanocomposite film is flexible, transparent and conductive which can be connected to the circuit on demand via light acting as an electrical switch. We believe it can be combined with various transparent electronic devices to further expand its applications.



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

Oral Presentation of Young Material Chemists

Room 322, THU 09:07

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Morphology-retained photo-conversion reaction of anthracene single crystal: a new approach for organic heterostructures

Jinyoung Koo^{*}, Hee Cheul Choi^{*}

Department of Chemistry, Institute for Basic Science, Pohang University of Science and Technology, Korea

The morphology of organic single crystal heavily affects its optical and electrical properties as these properties are determined by molecular arrangements in the crystal, and the morphologies generally reflect the molecular arrangements. In this presentation, we report the solid-state photo-conversion reaction of disk shape anthracene (**AN**) crystal into 9,10-anthraquinone (**ANQ**) and dipara-anthracene (**DPA**) crystals with the original crystal morphology retained. It should be noted that it is difficult to obtain such disk shape **ANQ** and **DPA** crystals by conventional crystallization methods, but they were realized by photo-conversion reaction of disk shape **AN** crystal. Time-dependent observation revealed the reaction mechanism as the photo-oxidation proceeded from the edge of the **AN** crystal due to oxygen diffusion while photo-dimerization occurs randomly. Interestingly, the electrical conductivity of photo-converted 9,10-anthraquinone (**PC-ANQ**) crystal is about five orders of magnitude higher than that of the starting **AN** crystal while the photo-converted dipara-anthracene (**PC-DPA**) crystal exhibits a decreased conductivity. Structural contributions to electrical conductivity differences were investigated by X-ray diffraction (XRD) and single crystal phase indexing, we revealed that the solid-phase photoreaction could induce molecular rearrangement. The remarkable advantage of solid-state photochemical reaction is that the reaction area is readily controlled by light irradiation area. By taking this advantage, we found a new approach to synthesize the lateral heterostructures (**AN-ANQ**, **AN-DPA**, and **ANQ-DPA**) by area-selective photoreaction using a chrome photomask.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:14

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Unprecedented Control of Organic Polyhedral Molecular Crystals by Solvent Addition Order and Anti-solvent Molecular Geometry

Yohwan Park, Hee Cheul Choi^{1,*}

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

¹*Department of Chemistry, CALDES, Pohang University of Science and Technology, Institute for Basic Science, Korea*

In this presentation, we report the elucidation of the effect of anti-solvent molecular geometry and solvent addition order on the determination of the morphology of molecular crystal toward the formation of organic polyhedral molecular crystal morphology without using chemical additives. Although organic polyhedron is greatly important for achieving desirable properties, its efficient growth without any additives remains as a big challenge. To achieve this, we developed the reverse anti-solvent crystallization (*r*-ASC) method [1] and revealed that the molecular geometry of anti-solvent and its addition order play a critical role in determining the morphology of the final molecular crystal. For this, we studied for tetra (4-aminophenyl) porphyrin (**TAPP**) in ethanol/xylene binary solvent system. When the *r*-ASC process was done for the **TAPP**, rod-, disk- and cube-shaped **TAPP** crystals were grown by using *o*-, *m*- and *p*-xylene anti-solvents, respectively. The three kinds of crystals have totally different crystal structures as confirmed by single crystal X-ray diffraction. The results show the three kinds of xylene geometry could affect numerous interacting sites to **TAPP** and the crystal growth direction because to the different solvent geometry alters the local supersaturation environment. These results are meaningful because not only it opens up a way to for the realization of quite rare organic polyhedral crystals, but also it would provide versatile opportunities for fundamental crystallization studies. Reference[1] Park, Y.; Hong, M.; Koo, J. Y.; Lee, M.; Lee, J.; Moon, D. J.; Sohn, S. H.; Joo, T.; Lim, W. T.; Lim, H.; Choi, H. C. *Sci. Rep.* **2017**, *7*, 2582.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:21

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Rapid and highly Efficient Synthesis of a Scalable Two-Dimensional Covalent Organic Framework (COF) by Photon-assisted Imine Condensation Reaction on the Water Surface

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An atomically thin two-dimensional (2D) covalent organic framework (COF) was successfully synthesized via photon-assisted imine condensation reaction within 1 h from the highly uniform and homogeneous precursor solution layer floating on the water surface. The polarity optimization of the precursor solution was the key for the successful formation of the high quality two-dimensional COF (2D COF) because only the precursor solution made of polarity-controlled solvents allows the ideal floating on the water surface. The polarity-controlled solution not only prohibits the agglomeration of the organic precursors on the water surface, but also facilitates the wafer scale and layer number-controllable synthesis of 2D COF. Our film shows uniformly porous, layered structure, of which layers align along the out-of-plane direction, as confirmed by atomic force microscopy (AFM), transmission electron microscopy (TEM), and grazing-incidence wide-angle X-ray scattering (GIWAXS). In addition, we successfully fabricated pi-COF thin film transistor-type electronic devices which show quite prompt electrical responses to photo and water vapor exposure. We believe that our findings would contribute to the development of novel synthetic methods of various two-dimensional COF films on the water surface and provide a new insight into practical applications of COF films in electronics.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:28

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

High Performance Flexible Organic Field Effect Transistor

Geonho Kim, Jiwon Kim*

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Recent years, organic based field effect transistor has been actively studied since organic semiconductors are biocompatible, easy to fabricate large area and low in cost.[1] Furthermore, organic semiconductors are flexible compared to conventional semiconductors (such as Si or GaAs etc.); therefore, they are applied in various devices such as wearable devices, robotics, and portable electronics, etc. However, they still suffer from relatively low field effect mobility which is important in transistor performance. Here, we report high performance flexible organic field effect transistor (OFET) using Li doped poly(3-hexylthiophene-2,5-diyl) (P3HT) as channel, ion gel as gate and Au nanoflakes as electrodes. Li doped P3HT has relatively high carrier density and mobility (up to $1.4 \text{ cm}^2/\text{V}\cdot\text{s}$),[2] whereas ion gel has high carrier conductivity and high stability in ambient environment. Ion gel is also easy to fabricate nano/micro patterns on large area. Also, Au nanoflakes can be deposited onto flexible substrate maintaining good conductivity upon mechanical deformation. In sum, our flexible organic field effect transistor showed high performances (high mobility, stability, short response time and high ON/OFF ratio) suggesting its potential to be applied in various wearable electronic devices. Reference[1] Kim et al. Science advances, 2017, 3.9: e1701114.[2] Guo et al. Journal of Materials Chemistry A, 2014, 2.34: 13827-13830.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:35

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Controlled Restacking of Inorganic Nanosheets to Improve their Electrode Performance for Sodium Ion Batteries

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The stacking structure of layered material is important for optimizing its electrode property because of its profound effect on ion diffusion into the lattice. In this research, the restacked structure of exfoliated MnO₂ nanosheet can be controlled by adjusting the concentrations of tetramethylammonium (TMA⁺) and intercalant alkali metal ions. Powder X-ray diffraction and X-ray adsorption spectroscopic (XAS) analyses clearly demonstrate the maintenance of the original layered structure of MnO₂ nanosheet upon the restacking process. According to N₂ adsorption-desorption isotherm analysis, the porosity of the restacked MnO₂ nanosheets can be tailored by changing the restacking condition. Of prime importance is that the increase of TMA⁺ concentration leads to the improvement of the discharge capacity of restacked MnO₂ nanosheets for sodium ion batteries, indicating the beneficial effect of the high concentration of TMA⁺ ions on electrode performance. The present study underscores that the fine-control of stacking condition can provide an effective way of optimizing the pore structure and electrode functionality of restacked metal oxide nanosheets.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:42

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Time-Controlled Nanoscale Delivery System

Jihyeon Park, SeoYeah Oh, Dongjun Kim¹, Wonsik Lee, Geonho Kim, Jiwon Kim*

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Many reactions, especially in vivo, are time-dependent since reactants degrade or change over time. Therefore, delivering cargoes at desired time points and positions in nanoscale is necessary and injection at different time points is possible. However, it is difficult to spatio-temporally control the transmission of cargoes especially within short period time because they proceed with random walk motion. Thus, nanomotors – which the velocity can be controlled in nanoscale fluid systems – can be good candidate. Since controlling with two different external driving force on the same type of nanomotor is challenging to precisely control the velocity, herein, we designed two (or more) types of nanomotor which can travel at different speeds under the same applied stimuli. The nanomotors were composed of gold head – silver flexible filament – nickel tail encapsulated with N-isopropylacrylamide (NIPAm) based hydrogel. The difference in speed was controlled by adjusting the length of each compartment whereas the cargo releasing time was regulated by optimizing the thickness of encapsulating hydrogel. Our nanomotor based nanoscale delivery system can control the delivery time down to a few minutes, which can possibly increase the efficiency of multiple drugs or gene editing (where the cargoes easily degrade/denature) and also be used in molecular communications for transmitting information through (bio)materials. We believe the spatio-temporally controlled nanoscale delivery system will broaden the range of application areas of nanomaterials by enhancing the spatial and temporal accuracy in delivering cargoes in nanoscale.

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:49

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Fruit browning mimetic protective coating for extreme environment endurance at the biological interface

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For a living organism, maintaining stability between the internal environment and the external environment is an important factor for survival. Therefore, the surface of an organism acts as a barrier that is usually satisfactory for most external environments, but extreme environments such as vacuum space can cause these natural barriers to be insufficient. We propose a fruit browning chemistry mimetic protective coating at the biological interface to be able to withstand extreme environment. The coating is achieved by the aerobic oxidation of the pyrogallol (PG) moiety, which is abundantly found in plant polyphenol derivatives that result fruit browning on air-exposed surface. In our study, enzyme-mediated aerobic oxidation of pyrogallol in fruit browning process was successfully replaced to pH-induced aerobic oxidation followed by Michael-type reaction with the amine-rich polymer, polyethylenimine (PEI). We applied this coating to the surface of various soft matters such as hydrogels, polymeric microbeads, plant leaves, and soft tissues for electron microscopic imaging. The coating protected these soft matters from dehydration and thermal melting in ultra-high vacuum condition with the electron beam exposure in the scanning electron microscopy (SEM). Surprisingly, dehydration protection makes the surface conductive, so the metal sputtering process, which is mandatory for organic specimens for SEM imaging, was not needed. Therefore, fruit browning mimetic coating allows simple and rapid analysis of biological specimens without conventional multiple sample preparation steps (e.g., dehydration in gradient ethanol solutions and metal sputtering).

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

Oral Presentation of Young Material Chemists

Room 322, THU 09:56

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Reversible Switching Nanoscale Sensor for Real Time Tracking

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In order to accurately – selectively and sensitively – detect target material within a small space (e.g. blood vessel), a nanoscale sensor with high density integration is required. Nanomaterial is a good candidate since it has many detection sites in a localized space; however, reversible reaction between target material and detection sites are still rare with short response time. Herein, we designed nanoscale sensors via gold nanoparticles (AuNPs) functionalized with 11-mercaptopundecanoic acid (MUA) and N,N,N-trimethyl 11-mercaptopundecyl ammonium (TMA). MUA and TMA ligands (or mixed) functionalized AuNPs (MUA/TMA AuNPs) can change surface charges according to surrounding pH change which can be easily recorded in real time by ζ -potential (ca. 20 mV in acid condition of pH ~ 3.0 and ca. -30 mV in basic condition of pH ~ 11.0). For real time detection, dilution and separation models were designed in order to minimize accumulation of information particles around the sensor. As a result, we could develop reversible switching nanoscale sensor which can read out dynamic signals in real time giving us more accurate information and can possibly be applied in nanoscale communication systems.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:03

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Electospun Fibrous PCL and PLGA mats incorporated with AuRD for Photothermal therapy

Hojun Seo, Eunmi Im, Geondae Moon*

Korea Institute of Industrial Technology, Korea

Photothermal therapy (PTT) based on near-infrared (NIR) light has been attracting huge attention to replace conventional treatments for cancer therapy because of its minimal invasiveness and high selectivity. An irreversible damage can be done to tumor cells by using photothermal agents that can absorb NIR light and dissipate the absorbed energy to heat in the cells. Nevertheless, the treatment of only PTT is incapable of achieving satisfactory therapeutic effect because of heterogeneous distribution of heat generated within the tumor. In addition, survived cancer cells after the treatment can induce cancer metastasis or recurrence. In this presentation, we introduce new fibrous systems with photothermal agents designed from a combination of PTT and chemotherapy. The first system consists of polycaprolactone (PCL) including Au nanorods as a photothermal agent to demonstrate the optimal heat generation condition by changing the absorbed wavelength. The photothermal efficiency varies based on aspect ratio of Au nanorods showing different absorption efficiency. The second system contains poly(D,L-lactic-co-glycolic acid) (PLGA) hollow fibers encapsulating an anticancer drug in their core, accompanied by shell with Au nanorods to prevent an undesired passive release of the drug molecules. On exposure to NIR light, the photothermal agent entrapped in the shell generates heat to raise the local temperature of the fibers. Above a glass transition (T_g), the polymer chains will be mobile, which enlarges free volume in size within the shell and consequently results in a rapid release of the drug. The segment of the chains will freeze by the inactivity of the photothermal agent when NIR light is turned off, which terminates the drug release. A repeated and accurate release of the drug is possible in an on-demand manner through the segmental switching of the polymer chains in response to the on-off operation of NIR light. Therefore, the anticancer activity can be enhanced by the hyperthermia effect from the photothermal agent.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:10

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Precisely Shaped, Uniformly Formed Gold Nanocubes with Ultrahigh Reproducibility in Single-Particle Scattering and Surface-Enhanced Raman Scattering

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Synthesizing plasmonic nanostructures in an ultraprecise manner is of paramount importance because the nanometer-scale structural details can significantly affect their plasmonic properties. Au nanocube (AuNCs) have been a highly promising, heavily studied nanostructure with high potential in various fields, but an ultraprecise synthesis from 10 to 100 nm in size over a large number of AuNCs has not been well established. Precisely structured AuNC-based studies for a highly reproducible, quantitative plasmonic signal generation [e.g., quantitative surface-enhanced Raman scattering (SERS)] are needed for reliable use and exploration in the beneficial properties of AuNCs. Here, we developed a strategy for AuNC synthesis with the desired size and shape, ranging from 17 to 78 nm particularly with highly controlled corner sharpness, by precisely controlling the growth rate of different facets and AuNC-specific flocculation which enabled ultrahigh yields ($\sim 98\text{--}99\%$). Importantly, the precisely shaped AuNCs can scatter light in a spectrally reproducible manner, and the SERS enhancement factors (EFs) for the AuNC dimers are very narrowly distributed (the EFs of 72 nm sharp-cornered cube dimers have a distribution within 1 order of magnitude). Our results pave the paths to ultrahigh yield synthesis of metal nanocubes with a precise size and shape and offer single-particle-level spectral controllability and reproducibility over a large number of particles.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:17

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Unexpected Finding of Pore Blockage & Local Graphitization of Si@C Yolk-Shell Structure during Magnesiothermic Reduction

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As current electronic devices need more capacity and long-lived energy storage, new materials that possess more energy storage are of highly desirable. Silicon presents capacity of 3580 mAh/g as anode material for lithium-ion batteries (LIBs), of which capacity is much higher than the capacity (372 mAh/g) of current graphite anode; thus it has been believed as a next-generation anode material for LIBs. Silicon anode suffers from several technical issues, however, which are of severe volume change up to 400 % during cycling and low electric conductivity. In addition, at the first cycle, silicon reacts excessively with the electrolyte to generate solid-electrolyte interface layer (SEI layer) due to volume expansion, which reduce the coulombic efficiency (CE), eventually resulting in lower the capacity of the battery. In order to compensate these disadvantages, the Si@C yolk-shell structure has been designed via various ways, among which magnesiothermic reduction of SiO₂@C composite to prepare Si@C yolk-shell structure has been of great interest in. Herein, we first report that complete pore blockage and local graphitization of carbon shell were identified during magnesiothermic reduction, which has not been reported so far. The microporosity of carbon shell was completely blocked after magnesiothermic reduction, determined by nitrogen sorption measurement. In addition, local graphitization of carbon shell was observed under TEM analysis and Raman analysis also supported the increase of graphitization degree. Such unexpected finding could be ascribed to the exothermic reduction nature of magnesiothermic reduction, resulted in graphitization and consequent pore blockage of carbon. As prepared Si@C yolk-shell structure exhibited outstanding capacitance of 1500 mAhg⁻¹ (@100 cycles) with stable long term stability and prominent rate performance.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:24

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Inorganic-Organic-Polymer Hybrid Bead as the Nutraceutical supplement with Essential Minerals and Vitamin

HyeonJu Ryu, Goeun Choi, Jin-ho Choy*

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We have designed and prepared a new hybrid composed of calcium alginate and metal hydroxide containing Mg^{2+} , Zn^{2+} , and Cr^{3+} as a mineral supplement for diabetic patients according to the recommended daily intake of nutrient minerals by FDA. As well documented, the deficiency of essential minerals such as Ca^{2+} , Mg^{2+} , Zn^{2+} and Cr^{3+} , and vitamin B₆ (VB₆) are causing various new cases of diabetes mellitus type II. So attempts have been made to prepare a mixed metal hydroxide (MMH) containing essential mineral ions by co-precipitation method. And it was then further dispersed in an aqueous solution of alginate containing VB₆, and thus prepared suspension was finally added to an aqueous solution of CaCl₂ to form calcium alginate bead hybridized with MMH nanoparticles and VB₆ as the final product (VB₆-MMH-calcium alginate). The chemical formula of MMH was determined to be $Mg_{0.988}Zn_{0.011}Cr_{0.001}(OH)_2$ as confirmed by ICP-AES analysis, which was well consistent with the theoretical one. According to the SEM and EDS studies, the crystal structure and shape of MMH nanoparticles were found to be thin and plate-like with a homogeneous size distribution of ~100 nm, those which were rather uniformly distributed in the beads. According to the *in-vitro* release profiles, the VB₆ molecules from VB₆-MMH-calcium alginate bead were released out only 37.8 % after 2 hours at pH 1.2, but ~80 % within 2 hours at pH 6.8, and gradually reached to ~98 % after 6 hours due to the pH dependent swelling behaviour of alginate polymer. In addition, the chemical stability test for intact VB₆ and VB₆-MMH-calcium alginate bead was also performed at 25 ± 2 °C in 60 ± 5 % humidity for 2 months based on the guideline of Korean FDA. After 2 months exposure, the VB₆ content for the former was strongly reduced down to 30 %, but that for the latter was remained almost unchanged to be 97 % indicating its enhanced stability. Therefore, we suggest that the present hybrid system, VB₆-MMH-calcium alginate bead, can be an excellent nutraceutical supplement for diabetic patients.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:31

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Soft Chemical Route to Single Molecular Layered g-carbon nitride

Huiyan Piao, Goeun Choi, Jin-ho Choy*

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Graphitic carbon nitride (g-C₃N₄) has received a great attention not only due to its high chemical and thermal stability, but also its various applications like visible light harvesting photocatalyst, metal-free catalyst and reactive template in nitridation reaction. In addition, its single sheet has attracted great research attention, due to the fact that its single layered molecular structure is very similar to the graphene except tri-angular hole, giving rise to a remarkable enhancement of specific surface area. It is, however, a challenging task to prepare chemically well-defined single sheet of g-C₃N₄. In the present study, single layered g-C₃N₄ could be obtained from the bottom-up process based on the polycondensation reaction of cyanamide as a g-C₃N₄ precursor, in the interlayer space of 2D aluminosilicate as a 2D nanoreactor (Mica). The single layered g-C₃N₄ can finally be separated from thus prepared g-C₃N₄-Mica nanohybrid, since the aluminosilicate matrix can be dissolvable under an acidic condition. Each reaction step to single layered g-C₃N₄ from cyanamide confined in 2D nanoreactor was monitored by X-ray diffraction, FT-IR, UV-Vis, XPS and EELS analyses. According to the AFM analysis, the average topographic height of as-prepared single layered sheet was determined to be around 0.5 nm, which is almost equal to the thickness of a single layer g-C₃N₄. Finally, the crystal structure of single layered g-C₃N₄ in an atomic level was further confirmed by low dose Cs-corrected high-resolution transmission electron microscopy (Cs-HRTEM). The single layered sheet exhibited an ordered structure of well-defined hexagonal symmetry with cavity formed by in-plane encirclement of three adjacent heptazine units. It is, therefore, concluded that the present soft chemical route to g-C₃N₄ single sheet can give rise to atomically well-defined phase consistent made of tri-s-triazine building blocks.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:38

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Enhanced Mechanical and Flame Redarding Properties of ABS Nanocomposites with Organo-Clays

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Acrylonitrile–butadiene–styrene copolymer (ABS) nanocomposites with cationic and anionic clays were successfully synthesized via a solution blending method. Cationic clay (Fluoro-mica; ME) and anionic clay (layered double hydroxide; LDH) were modified with hydrophobic molecules such as cetyltrimethylammonium (CTA) and stearate (SA), respectively, for improving the compatibility with hydrophobic ABS. All the ABS nanocomposites in the present study were prepared by changing the synthetic parameters such as the content of organoclay, the volume of solvent, and the sonication condition. In ABS nanocomposites containing SA-LDH, the (001) XRD peaks originating from SA-LDH were not observed, indicating that SA-LDH layers were fully exfoliated and homogeneously dispersed within ABS matrix. On the other hand, the (001) ones for ABS nanocomposites containing CTA-ME without any sonication treatments were remained, but shifted to a low 2θ angle due to the fact that the hydrophobic ABS molecules were further intercalated into the interlayer space of CTA-ME giving rise to an increase of basal spacing. However, the (001) peaks for ABS/CTA-ME nanocomposites were completely disappeared upon sonication, indicating that CTA-ME layers were exfoliated and homogenously dispersed in ABS matrix. According to the thermogravimetric analysis, the thermal stability of ABS nanocomposites was gradually improved by increasing the content of SA-LDH. The ABS nanocomposites containing well-dispersed organoclays showed ~25 % enhancement of mechanical properties, such as elastic modulus and tensile strength, upon increasing the content of CTA-ME, compared to intact ABS surely due to the high dispersity of organo-clay nanosheets in ABS matrix.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:45

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

Artesunate-Zinc Basic Salt Nanohybrid as a Novel Antimalarial Drug; Oral and Intravenous Administrations

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Artesunate (AS) is known as a water soluble anti-malarial drug (52.2 mg/L), but its bioavailability is rather low due to its limited aqueous solubility. In order to overcome this problem, a novel drug delivery system with hydrophilic function was suggested and demonstrated by intercalating AS into inorganic nano-vehicle like zinc basic salt (ZBS) via co-precipitation method. According to the powder x-ray diffraction analysis, the basal spacing of AS-ZBS nanohybrid was determined to be 2.88nm, indicating that AS molecules were successfully incorporated into the interlayer space of 2D ZBS host lattice. And the intracrystalline structure and molecular orientation of AS in the lattice could be confirmed by comparing the experimental 1-D electron density mapping result from the (00*l*) XRD data with the calculated one from the structure model of AS-ZBS, and partly by TEM analysis as well. The FT-infrared spectra revealed that AS molecules were deprotonated and electrostatically incorporated between cationic zinc hydroxide layers without any structural modifications. According to the CHNS, TG and HPLC analyses, the AS content in AS-ZBS was determined to be 45.8 wt%. In order to hold down dissolution and burst release of AS from AS-ZBS in a gastric juice condition, the AS-ZBS was further coated with an enteric coating polymer like Eudragit[®] L100 (AS-ZBS-L100), which dissolves in the basic environment of the intestines, for controlling the rate of drug release with respect to the pH values in the digestive tract. As expected, the AS-ZBS-L100 nanohybrid showed a remarkable increase in the release rate of AS in a simulated intestinal condition (pH 6.8) compared to the intact AS. In addition, we have performed in-vivo pharmacokinetic study in rats via oral administration in order to compare the absorption of AS out of the AS-ZBS-L100 nanohybrid with that of intact AS. Surprisingly, it was found that the former was ~6 times larger than the latter due to an enhanced solubility of AS thanks to the hybridization with hydrophilic ZBS. Therefore, AS-ZBS-L100 could be suggested as a promising drug delivery system for improving drug solubility and absorption. Additionally,

an attempt was made to encapsulate AS molecules into layered double hydroxide (LDH) for intravenous injection. All the in-vitro results including drug release behavior in the simulated body fluid will be demonstrated in-detail in this presentation.

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

Oral Presentation of Young Material Chemists

Room 322, THU 10:52

Chair: Jin Kuen Park (Hankuk University of Foreign Studies)

LVHR-SEM Images for Porous Carbons Replicated from Novel Geopolymer Template

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An attempt is made to demonstrate nanoporosity and nanomorphology of mesoporous carbons replicated from our porous geopolymer template with the low voltage high resolution scanning electron microscopy (LVHR-SEM). In this study, the SEM observation could be made not only for the porous geopolymer but also for the porous carbon with clear images on intra-wall pores, uniform cylindrical pores and packed nanowires. In addition, the CO₂ uptake capacity for this prepared porous carbon is carefully analyzed. Different from porous carbons conventionally prepared with porous silica template, which is in general synthesized from tetraethoxysilane (TEOS) as a silicon precursor, the present novel geopolymer template route to porous carbons is suggested not only to induce higher specific surface areas and larger pore volumes but also to provide a cost effective way of synthetic process compared to the conventional TEOS one. The porous geopolymer prepared from metakaolin (PG) is observed to be structured with hexagonal channels revealing unique and well-ordered mesopores of 7.20 nm as well as micropores, those which are connected with mesopores each other. The porous carbon rods (CPG) are effectively replicated from the PG template to form regularly packed and ordered structure with such high BET surface area (~ 1500 m²/g) and pore volume (~ 1.5 cm³/g) as demonstrated by such a high CO₂ uptake capacity of 26.3 mmol/g at 273k and 30 atm due to the presence of mesopores and micropores appropriately.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 09:00

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Effect of metal doping in the electronic structures of $M_2Au_{36}(SC_6H_{13})_{24}$ ($M=Pt, Pd$)

Minseok Kim, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Over the past decade, owing to their unique electronic structures with high chemical and thermodynamic stability, thiolate ligand-protected gold nanoclusters have been extensively studied. Recently, bimetallic gold nanoclusters have been reported, which represents a viable strategy to study the sensitivity of physical-chemical properties of the nanoclusters towards replacement of a single or few gold atoms by other metals. In particular, bimetallic $M_xAu_{38-x}(SR)_{24}$ nanoclusters ($M=Pt$ or Ag , SR =thiolate ligand) have been studied recently due to their different optical and electrochemical properties. In this poster, we report the stable bimetallic clusters ($[Pd_2Au_{36}(SR)_{24}]^0$ and $[Pt_2Au_{36}(SR)_{24}]^{2-}$) which showed different electronic configurations, by replacing the core Au atom with Pd and Pt. The highest occupied molecular orbital-lowest unoccupied molecular gap of $[Pd_2Au_{36}(SR)_{24}]^0$ determined by voltammetry was drastically decreased to 0.26 eV, but that of $[Pt_2Au_{36}(SR)_{24}]^{2-}$ was comparable with $[Au_{38}(SR)_{24}]^0$ (0.94 eV), indicating the electronic structures could be altered upon doping of the foreign metal. This result could be illustrated by their different electron configurations, that is $[Pd_2Au_{36}(SR)_{24}]^0$ cluster which has 12 electron exhibits remarkably different optical and electrochemical properties from those of the 14 electron $[Au_{38}(SR)_{24}]^0$ and $[Pt_2Au_{36}(SR)_{24}]^{2-}$.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 09:15

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Atomically Controlled Bimetallic Nanoclusters as Electrocatalysts for Hydrogen Production

Woojun Choi, Kyuju Kwak, Minseok Kim, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Hydrogen is widely considered as a clean and renewable energy carrier. Thus, identification of an efficient hydrogen evolution reaction (HER) electrocatalysts is one of the great challenging fields to replace the fossil fuel. Ligand protected Au nanoclusters exhibit distinctive electrochemical property and HER activity. The HER activity could be improved not only by doping of Pd or Pt to achieve thermoneutral binding step with H^+ ($\Delta G_H = \sim 0$ eV) but also by introducing proton rich ligand for fast proton relay from ligand to active site. In this presentation, we report electronic structures and catalytic properties of $Au_{25}(SR)_{18}$ and bimetallic $MAu_{24}(SR)_{18}$ ($M = Pt$ or Pd) nanoclusters ($SR =$ thiolate). The modified catalytic activities were demonstrated by linear sweep voltammetry and controlled potential electrolysis. HER turnover frequency (TOF) of hexanthiol (C_6S) protected $Au_{25}(C_6S)_{18}$ ($8.8 s^{-1}$ at -0.6 V vs. RHE) increased by doping of Pd ($13.0 s^{-1}$) and further enhanced by doping of Pt ($PtAu_{24}(C_6S)_{18}$, $33.4 s^{-1}$). Calculated ΔG_H by density functional theory supported the enhanced HER activities of Pd and Pt doped nanoclusters. The TOF of Pt-doped nanocluster could further increase by introducing carboxylate or sulfonate ligands reached to $100 s^{-1}$ at -0.6 V. Furthermore, Pt-doped nanoclusters catalyze hydrogen production from very low onset potential ($E_{onset} = -0.07$ V) due to matched reduction potential with proton (H^+/H_2) whereas Au_{25} showed mismatched reduction potential and higher E_{onset} (-0.20 V).

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 09:30

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Studies on the electrolyte enabling highly efficient performance of Li metal batteries

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Korea*

Graphite and silicon, which are representatively used as anodes of Li-ion batteries, seem to reach the saturation point regarding to relatively lower energy density of graphite-based Li-ion batteries and huge volume expansion causing rapid capacity fading of silicon-based Li-ion batteries for large-scale applications such as electric vehicles and grid energy storage. Thus, lithium (Li) metal has attracted great interest again as the next generation energy source to solve the urgent requirement for high-energy storage systems due to its high theoretical capacity (3800 mAh/g). Nevertheless, some issues such as Li dendrite growth possibly leading to short-circuit and thermal runaway and poor coulombic efficiency (CE) have still prevented the commercialization of secondary batteries using Li metal in spite of intense studies. Recently, the electrolyte which consists of superconcentrated imide salt and glyme solvent was suggested for the utilization of Li metal as anodes. This electrolyte showed great CE (> 98%) in repeated Li deposition/stripping processes in the previous report. In our study, a modified electrolyte named DS#1 is examined to exhibit an extraordinary CE (> 99%) and long life-time without short-circuit issue in Li-Li cycling. We further utilize DS#1 with the various cathodes and Li metal anode.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 09:45

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Controlled synthesis and characterization of Pd-based catalysts with enhanced electrocatalytic activity toward ORR/OER

Anh.T.N Nguyen, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Considering global energy scenarios, oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are the most important electrochemical reactions. An important concern in the scientific community to develop low-cost, active and stable ORR and OER catalysts is due to the fact that both Pt and Ir are expensive and rare. Alternatively, the design of highly active and stable catalysts using Pd and Pd-based nanomaterials has focused attention more recently due to the relatively high ORR activity, stability, greater abundance and almost half the cost of Pt. Thus, we report an efficient synthesis of size and shape-controlled Pd nanostructure in aqueous solution and their electrocatalytic activity for ORR. The proposed synthesis was examined using L-ascorbic acid as a reducing agent of Pd(II) in the presence of both a stabilizer and a capping agent such as Pluronic F127. The resultant Pd nanoparticles have different sizes, while their shapes can be controlled by using Pluronic F127 : halide anions (Cl⁻, Br⁻, I⁻) with different aspect ratios. On the other hand, iridium, as a second metallic element, is not only the best catalyst for the OER but also an excellent transition metal component to improve catalysis because it can form oxygen species on the surface at relatively low potentials. To lower the cost, several studies have focused on minimizing the use of Ir for improving the electrocatalytic activity of Ir-based nanomaterials. This presentation introduces a facile one-step process to synthesize highly interconnected nanoporous Ir-Pd alloys supported on carbon that exhibit excellent bifunctional electrocatalytic activities for both the ORR and OER with reasonable stability in alkaline electrolytes. The nanoporous Pd networks with crystalline {111} faces are shown experimentally to serve mainly as active sites for the ORR, whereas the Ir nanoparticles incorporated in the Pd nanoframe networks, where the optimized Ir : Pd ratio was 0.23 : 0.77 (n = 10), were responsible for the OER. Such three-dimensional architectures provide a high density of active sites for the oxygen electrochemical reaction and facilitate electron transport. More importantly, the nanoporous Ir-Pd alloy nanocomposites exhibited similar stability for the oxygen reduction reaction but superior catalytic activity to the commercial

Pd catalyst in alkaline solutions. In addition, the materials were also highly active for the oxygen evolution reaction, e.g., a small overpotential at 10 mA cm⁻² (1.628 V vs. reversible hydrogen electrode), making it a high-performance bifunctional catalyst for both the oxygen electrochemical reaction. Rotating ring-disk electrode measurements showed that the ORR and OER on the Ir-Pd catalysts proceeded predominantly through the desired 4-electron pathway. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 10:00

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

High power density thermoelectrochemical cell for harvesting low-grade heat

Kyunggu Kim, Hochun Lee*

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

Thermal energy is an attractive energy source considering its abundance and accessibility. A thermoelectric (TE) device can directly convert waste heat into electricity by the Seebeck effect. A thermoelectrochemical cell (TEC) is an electrochemical analogue of the TE device. The TEC consists of two identical electrodes immersed in an electrolyte, and generates the electricity by the temperature dependence of the free energy difference between reactant and product. Early studies investigated the TECs based on $\text{Fe}(\text{CN})_6^{3-/4-}$ redox couple, which employed Pt electrodes and aqueous solvent. Recently, most research into TEC with $\text{Fe}(\text{CN})_6^{3-/4-}$ redox mediator has focused on enhancing power performance to utilize sophisticated carbon materials having high specific electrode area. However, this approach cannot be expected to produce significant enhancement of TEC performance. Thus, further investigation of new electrolyte system with high Se and low electrochemical overpotential is encouraged. An important issue for present TEC is to connect individual cells in series in order to obtain high voltage in practical aspect. Pioneers combined the cells which exhibit negative and positive Se, $\text{Fe}(\text{CN})_6^{3-/4-}$ and $\text{Fe}(\text{SO}_4)/\text{Fe}_2(\text{SO}_4)_3$ electrolytes. However, $\text{Fe}(\text{SO}_4)/\text{Fe}_2(\text{SO}_4)_3$ electrolytes have relatively poor output voltage and current properties compared to those of $\text{Fe}(\text{CN})_6^{3-/4-}$ redox system, which limits the achievable performance for the TEC array. Here, we elucidated a novel electrolyte system for the TEC, which shows a positive Se. First, we investigated the influence of the electrolyte composition on the output voltage and power performance. Subsequently, series connected TEC was facilitated with optimum electrolyte and conventional 0.4 M $\text{Fe}(\text{CN})_6^{3-/4-}$ electrolyte.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 10:15

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Electrochemical fabrication of gold nanoparticle/reduced graphene oxide hybrid nanocomposite modified electrodes for electrochemical biosensing applications

Chang-Seuk Lee, Da Eun Oh¹, Seungjoo Jang², Tae Hyun Kim*

Department of Chemistry, Soonchunhyang University, Korea

¹*Chemistry, Soonchunhyang University, Korea*

²*chemistry, Soonchunhyang University, Korea*

We introduce the preparation of the hybrid nanocomposite-modified electrode consisting of reduced graphene oxide (RGO) and gold nanoparticles (AuNPs) using the one-step electrochemical method. RGO/AuNPs nanocomposite was formed on a glassy carbon electrode by the co-reduction of GO and Au³⁺ using the potentiodynamic method. The RGO/AuNPs nanocomposite-modified electrode was produced by subjecting a mixed solution of GO and Au³⁺ to cyclic sweeping from -1.5 V to 0.8 V (vs. Ag/AgCl) at a scan rate 10 mV/s for 3 cycles. The modified electrode was characterized by scanning electron microscopy, Raman spectroscopy, contact angle measurement, electrochemical impedance spectroscopy, and cyclic voltammetry. The AuNP/rGO modified electrode was used as an electrochemical biosensor for the simultaneous and individual detection of dopamine (DA), ascorbic acid (AA), and uric acid (UA). The modified electrode shows high selectivity towards the determination of DA, AA, or UA in the presence of potentially active bioelements. The AuNP/rGO modified electrode was also functionalized with c-kemptide for protein kinase A (PKA) activity assay by electrochemical impedance spectroscopy. The PKA activity assay was successfully demonstrated utilizing the fabricated AuNP/rGO modified electrodes. Since this fabrication method utilizes only voltammetric scanning, it should be readily accessible for electrochemical biosensors for various applications.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 10:30

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Amorphous NiOOH catalyst Coupled V2O5/BiVO4 Inverse Opal Heterojunction Photoanodes for Improved Solar Water Oxidation

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

Photoelectrochemical water splitting (PEC) into hydrogen and oxygen using photocatalyst coupled electrocatalysts could potentially address the large-scale energy needs of future societies. The viability of this approach with rational design on porous inverse opal constructed V2O5 photocatalyst coupled semiconductor BiVO4 heterojunction accompanied by efficient amorphous NiOOH for PEC water splitting is systematically explored. V2O5 IO film shows low photocurrent density due to the high-density surface states and short hole diffusion length that stimulate the high recombination of the photogenerated charges occurring in the bulk and surface states. V2O5@BiVO4 inverse opal structure increases the light absorption efficiency via ordered uniform pathway, control surface light reflection and increasing light scattering in all direction. The deposition of the BiVO4 layer on the photoanode to create a junction as well as to reduce the charge recombination at the surface trapping states of V2O5 IO film. Further, NiOOH layer was electrodeposited on V2O5@ BiVO4 IO film to enhance the PEC performance at a low potential region.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 320, THU 10:45

Chair: Yang-Rae Kim (Kwangwoon Univeristy)

Methanol dehydrogenation reaction at Au@Pt catalysts: Insight into the methanol oxidation

Hwakyung Jeong, Jongwon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

The methanol oxidation reaction (MOR) on Pt has received great attention because of its importance in the development of fuel cells. It is widely accepted for MOR on Pt that the methanol molecule is first adsorbed on Pt, and then adsorbed methanol is further electrochemically reduced via different pathways; CO pathway or non-CO pathway. During the MOR involving CO as intermediates, methanol dehydrogenation reactions should be preceded to produce COads. The methanol dehydrogenation reaction (MDHR) is important for elucidating the reaction mechanism of MOR. Recently, bimetallic Au-Pt catalysts were developed as efficient MOR electrocatalysts. In this work, the MDHR on Pt layers modified on Au surfaces using in-situ surface-enhanced Raman scattering (SERS) was investigated. The Pt layers with different the coverage and thickness on dendritic Au rod surfaces were fabricated using the self-terminating electrodeposition. The rate of MDHR at OCP and applied potential was examined by SERS techniques on different DAR@Pt(n) surfaces. Based on the SERS results, the effect of COads generated from the MDHR on the CV measurement of MOR was examined.

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

Oral Presentation for Young Scientist in Environmental and Energy Chemistry

Room 306A, THU 09:10

Chair: Dongwook Kim (Korea Military Academy)

Core Metal in MAu₂₄(SR)₁₈ Nanocluster(M=Au, Pt) Controls the Products Selectivity in Electrocatalytic CO₂ Conversion

Yongjin Lee, Hoeun Seong, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Gold nanoparticles have been studied extensively as an efficient electrocatalyst for CO₂ conversion. However, the electrochemical CO₂ conversion on gold nanoparticles typically requires large overpotentials and the reaction products are a mix of major and minor products, including CO and hydrogen. In this poster, we report that the product selectivity can be controlled by the core dopant of MAu₂₄(SR)₁₈ (M= Au, Pt), where SR is 1-hexanethiol. Linear Sweep Voltammetry studies show that the onset potential of CO₂ reduction catalyzed by Au₂₅(SR)₁₈ is significantly different from that by PtAu₂₄(SR)₁₈. Furthermore, constant potential electrolysis on electrodes modified with these clusters exhibits drastically different product selectivity. That is, whereas CO is predominantly produced on Au₂₅(SR)₁₈ with a selectivity higher than 90 %, nearly 75 % H₂ is produced on PtAu₂₄(SR)₁₈. Density functional theory (DFT) calculations show that the product selectivity appears to be closely related with the adsorption energies of the reactants, i.e., CO₂ and proton on the cluster catalyst.

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

Oral Presentation for Young Scientist in Environmental and Energy Chemistry

Room 306A, THU 09:35

Chair: Dongwook Kim (Korea Military Academy)

Developing a highly sustainable photocatalyst for outdoor air purification by hydrophilic surface modification of TiO₂

Saqlain Shahid, Young Dok Kim^{1,*}

Chemistry, SungKyunKwan University, Pakistan

¹*Department of Chemistry, Sungkyunkwan University, Korea*

Many TiO₂ based photocatalysts are being used in various ways for indoor and outdoor air purification now a days. The stability of these photocatalysts is the prime issue for their application because excess of contaminants from outdoor atmosphere deactivate the surface of the photocatalysts quite easily. Particularly the oil contaminants are hard to clean when exposed to surface because TiO₂ surface has good hydrophobicity. In current work by coating PDMS thin layer and subsequent heat treatment under vacuum conditions we modified the surface of commercially available TiO₂ (P-25) into more hydrophilic. The surface modified TiO₂ showed enhanced hydrophilicity attributed to the hydrophilic functional groups (e.g., C=O, C-OH, SiO_x) on the surface. Thus, oil contaminants on the surface could be effectively washed off with water hence sustaining clean surface. We evaluated UV light driven photocatalytic activity of hydrophilic surface modified TiO₂ towards degradation of acetaldehyde (one of the common air pollutants) under different humidity conditions. By increasing humidity, the absorption and photocatalytic activity of surface modified TiO₂ also increased whereas in case of bare TiO₂ both were decreased. But photocatalytic activities of bare as well as surface modified TiO₂ were suppressed above 33.6% of relative humidity just because of excessive humidity level. Finally it was revealed that as compared to bare TiO₂, the surface modified TiO₂ sustained higher photocatalytic activity for decomposition of acetaldehyde. We believe that our hydrophilic surface modified TiO₂ has much higher potential for long-term outdoor air purification.

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

Oral Presentation for Young Scientist in Environmental and Energy Chemistry

Room 306A, THU 10:10

Chair: Dongwook Kim (Korea Military Academy)

Effect of Inter-Enzyme Electrical Hindrance on Direct Electron Transfer at Synthetic Enzyme-Electrode Interface via Spatially Tunable-, and Nano-patterned Enzyme Electrode

Hyeonyeong Lee

Division of Environmental Engineering, Gwangju Institute of Science and Technology, Korea

Direct electron transfer (DET) in the enzyme-electrode system is crucial process for development of the alternative power sources of bioelectronics devices, biosensors, biofuel cells, etc. Efficient electrical communication in DET-based enzyme-electrode is important since DET efficiency of enzyme-electrode governs the performance of the devices. However, the enzymatic structure which the enzymatic active site is buried deep inside the protein matrix, obstruct the direct contact between enzymatic active site that is electron donor and electrode surface, causing poor electrical contact of enzymatic cofactor toward electrode surface. In addition to this, enzymatic agglomeration caused by protein-protein hydrophobic interactions could insulate DET during the immobilization of large amount of enzymes on the electrode. At the time, enzymatic cofactor which is electron donor for electrode can be hindered by non-conductive exterior of adjacent enzymes and ET at enzyme-interface will be prevented with its charge transfer resistance increased. Thus, in this study, the two factors that are ET distance and inter-enzyme steric hindrance, were considered to construct enzyme-electrode system with highly efficient DET process. Here, the synthetic glucose dehydrogenase (GDH) that DET capability and binding stability on the electrode. Furthermore, the influence of adjacent enzymes on DET efficiency was investigated on nano-patterned electrode, rendering nano-patterned enzyme-electrode where enzymes are spatially tuned on the electrode. The electrical performance of DET-based enzyme electrode was then estimated depending on condition of spatial tuning; less inter-enzyme insulation enabling favorable ET.

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

Oral Presentation for Young Scientist in Environmental and Energy Chemistry

Room 306A, THU 10:35

Chair: Dongwook Kim (Korea Military Academy)

Tuning the Electron Density of Aromatic Solvent for Stable Solid-Electrolyte-Interphase Layer in Carbonate-based Lithium Metal Batteries

Dong-Joo Yoo, Jang Wook Choi*

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

Lithium metal has been hailed as a key enabler of upcoming rechargeable batteries with high energy densities. Nonetheless, uncontrolled dendritic growth and resulting formation of a non-uniform solid-electrolyte-interface (SEI) layer constitute an ever-challenging obstacle in long-term cyclability and safety. So far, these drawbacks have been addressed mainly by using non-carbonate electrolytes based on their relatively mild decomposition under reductive environments. Here, we report toluene as a co-solvent of carbonate-based electrolytes for lithium metal anodes. The electron donating nature of the methyl group of toluene shifts the reduction of toluene prior to that of commonly used carbonate solvents, resulting in a more uniform and rigid SEI layer. Moreover, the polymerization process of toluene induces the decomposition of the bis(fluorosulfonyl)imide (FSI) anion in LiFSI salt to yield uniform distribution of lithium fluoride (LiF), and thus lowers an onset salt concentration in realizing the so-called 'high concentration effect' to 3 molar concentration, instead of 5 molar concentration as in typical electrolyte cases. This investigation reveals the usefulness of aromatic compounds in improving the stability of the SEI layer in lithium metal anodes, particularly by tuning the electron density of the benzene ring.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

High-transparent and good impact strength polycarbonate-polysiloxane copolymers process

Jieun Kim, Seong Hyen Heo*, Youngdo Kwon*

Chemical Research Laboratory, Samyang Corporation, Korea

This application relates to polycarbonate-polysiloxane copolymers having high transparency and good impact strength. Polycarbonate-polysiloxane copolymers of bisphenol A (BPA) and siloxane comonomers are known to have excellent impact resistance properties in comparison with BPA homopolycarbonates, especially at lower temperatures. Such materials have found commercial use in articles such as helmets, automobile parts, and many other applications requiring impact resistance and transparency. This polycarbonate-polysiloxane block copolymer is composed of at least one polycarbonate block, at least one polysiloxane block, and a bit of surface modifying agent that includes at least one polysiloxane segment. As the number of polysiloxane block increases, the impact resistance improves, but the transparency suffers, and vice versa. In order to improve transparency while obtaining good impact strength, a shorter unit of polysiloxane comonomer was used. The copolymer also exhibits improved hemocompatibility and therefore can be useful for a variety of articles that may contact blood.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Poly(carprolactone-hydroquinone) Oxalate (CQX) as ROS-sensitive degradable polymers

SeungYi Son, Heeju Kim, Hanbyul Jang, Byeongmoon Jeong*

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

PCL-OX (Polycaprolactone Oxalate) was reported as a fast degradable PCL and is a promising biodegradable material that solves the slow degradation problem of PCL over 2-3 years. In particular, degradation of the polymer was accelerated in the presence of hydrogen peroxide or reactive oxygen species (ROS). Therefore it can be used in a variety of biomedical applications where fast biodegradable polymers are needed. In continuation of the research, poly(carprolactone-hydroquinone) Oxalate (CQX) was synthesized by condensation polymerization using PCL diol 530, hydroquinone, and oxalyl chloride. Degradation of CQX was investigated as a function of ROS concentration.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Reactive oxygen species and thiol responsive micelles for efficient delivery of anti-cancer therapeutics

Young In Choi, Hyun-Chul Kim*

*Magnet-Controlled Materials Research Group, Daegu Gyeongbuk Institute of Science & Technology,
Korea*

Gemini amphiphile consisting of hydrophilic poly(ethylene glycol) (PEG) and hydrophobic poly(methionine) (PMT) with cystine disulfide spacers was synthesized and its micellar properties for thiol- or ROS (reactive oxygen species)-dependent intracellular drug delivery are described. The cleavage of cystine linkage in redox environment or the oxidation of methionine units in ROS environment caused the destabilization of micelles. Such redox- or ROS-triggered micellar destabilization led to enhanced release of encapsulated DOX (doxorubicin) to induce cytotoxicity against cancer cells. Therapeutic effects of the DOX-loaded micelles are demonstrated using KB cell line. This study shows that thiol and ROS dual responsive gemini micelles have potential use as a promising platforms for nano-drug delivery in various cancer therapies.

Poster Presentation : **POLY.P-4**

Polymer Chemistry

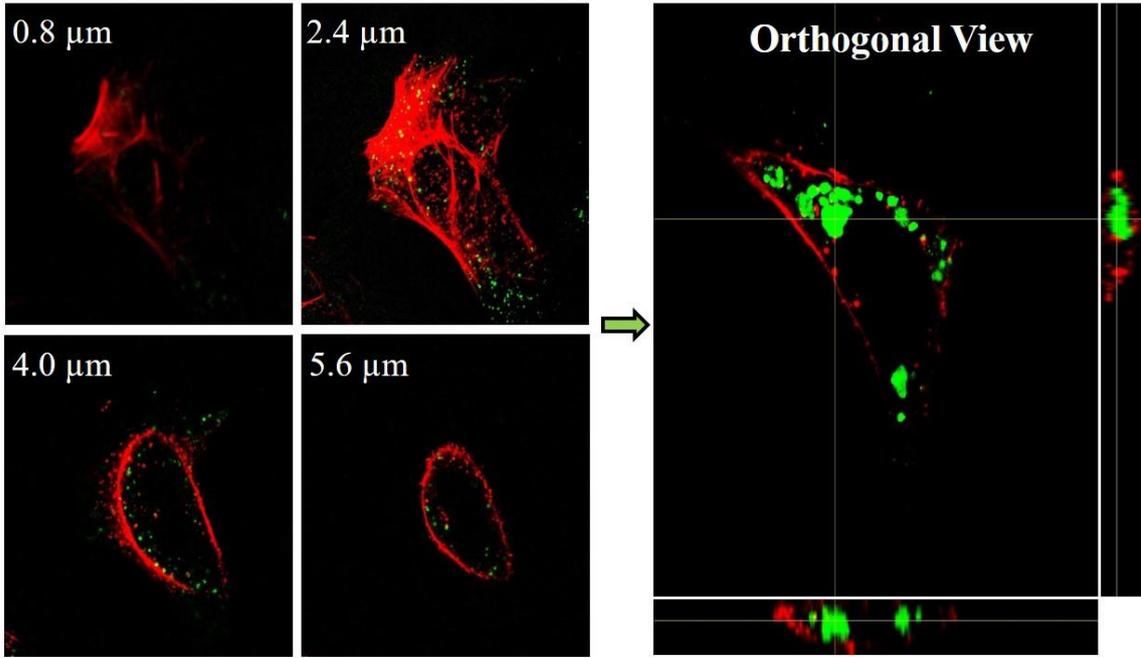
Grand Ballroom, THU 11:00~12:30

Double-Emulsion Nanoparticle Based on Biocompatible and Biodegradable L-Tyrosine Polyurethane for Efficient Gene Delivery

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 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 presynthesized from desaminotyrosyl tyrosine hexyl ester (DTH), and polyethylene glycol (PEG) through double emulsion method and used to evaluate their potential biological activities molecular controlled release and transfection studies. In order to evaluate cell adsorption and transfection of nanoparticles, two types of nanoparticles were prepared, the one from fluoresced using fluorescently labeled bovine serum albumin (FITC-BSA) to investigate cell adsorption, and the other from encapsulated with DNA-linear polyethylenimine (LPEI) complex to investigate the transfection efficiency in LX2 (human hepatic stellate cell), HepG2 (human liver cancer cell), MCF7 (human breast cancer cell). The morphology of these nanoparticles, which was confirmed both by microscope image and TEM, was a spherical shape with an average diameter of about 260 nm and 145 nm. The biodegradable nanoparticles showed the typical features of double emulsion. After 14 days, DNA in nanoparticles have been released from the LTU nanoparticles. Furthermore, a successful cellular uptake of LTU nanoparticles in hepatic stellate cells has been confirmed and high transfection efficiency also confirmed in LX2, HepG2 cells with check proper concentration of LPEI due to toxicity. These characteristics are ideal for gene therapy designed to transport and release a drug into the cytoplasm.



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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Luminescent Hierarchically Porous Polymer for Nitroaromatics Detection

Chinnadurai Satheeshkumar, Myungeun Seo^{1,*}

*Graduate School of Nanoscience and Technology, Korea Advanced Institute of Science and Technology,
Korea*

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

The detection of nitroaromatics is of great indispensable experimentation in the sense of security, health and environment issues. Fluorescence quenching is one of the fascinating approaches to recognize hazardous materials because of its intriguing advantages such as inherent sensitivity, high selectivity and easy handling. Hierarchically porous polymers combining micropores (

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Self-assembly of complex doubly grafted bottlebrush polymer from branched multiblock macromonomers

Jiyun Nam, Myungeun Seo*, Jeung Gon Kim^{1,*}

*Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology,
Korea*

¹Department of Chemistry, Chonbuk National University, Korea

The advancement of polymerization techniques extends complexity of polymer architecture from block copolymers followed by star polymers and graft polymers. As a class of graft copolymers, bottlebrush polymers are graft polymers containing grafted chains with every repeating unit. They exhibit high density of functional groups as well as extended conformation due to repulsion of the grafted chains. Janus-type bottlebrush polymer emerged as one of the bottlebrush polymer types in visualization for cylindrical Janus nanoobjects. Doubly grafted side chains attached along the backbone enables to achieve cylindrical Janus morphology type via intramolecular segregation of incompatible side chain. Here we explored synthesis of doubly grafted bottlebrush polymers (DGBP) via graft-through ring-opening metathesis polymerization (ROMP) of branched multiblock macromonomers (BMMMs) towards complex Janus-type bottlebrush polymers with two different surfaces. By utilizing single monomer unit insertion (SUMI) in the reversible addition-fragmentation chain transfer (RAFT) process, we will discuss synthesis of the BMMMs containing two, three blocks with different compositions. Characterization of complex Janus DGBP and their self-assembly behaviors will be also presented.

Poster Presentation : **POLY.P-7**

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Photoinduced Metal-Free Atom Transfer Radical Polymerization with Diverse N-aryl Phenoxazine

Gyeong Su Park, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

Atom transfer radical polymerization (ATRP) has been in the spotlight by far as a groundbreaking synthetic method. Using this process, the distribution of functional groups, molecular weight of polymers, polydispersity and others can be precisely regulated, whereby the polymers with a various structure also can be designed and manufactured. However, contamination of the polymer by the metal catalyst remains a challenge, which limit the use of the traditional ATRP method in electronic or biomedical applications. The drawback has spawned investigations into the development of organic catalysts for photo-controlled, metal-free polymerizations. Herein, we investigated the metal-free ATRP process mediated by light and catalyzed by organic photoredox catalysts. The organic photocatalyst was designed by diversifying N-aryl phenoxazine. We evaluated our newly discovered organic photoredox catalysts for metal-free ATRP using a series of monomers, initiators and solvents. Also, amphiphilic block copolymer was prepared using this method to form micelles, providing a basis for the biomedical applications.

Poster Presentation : **POLY.P-8**

Polymer Chemistry

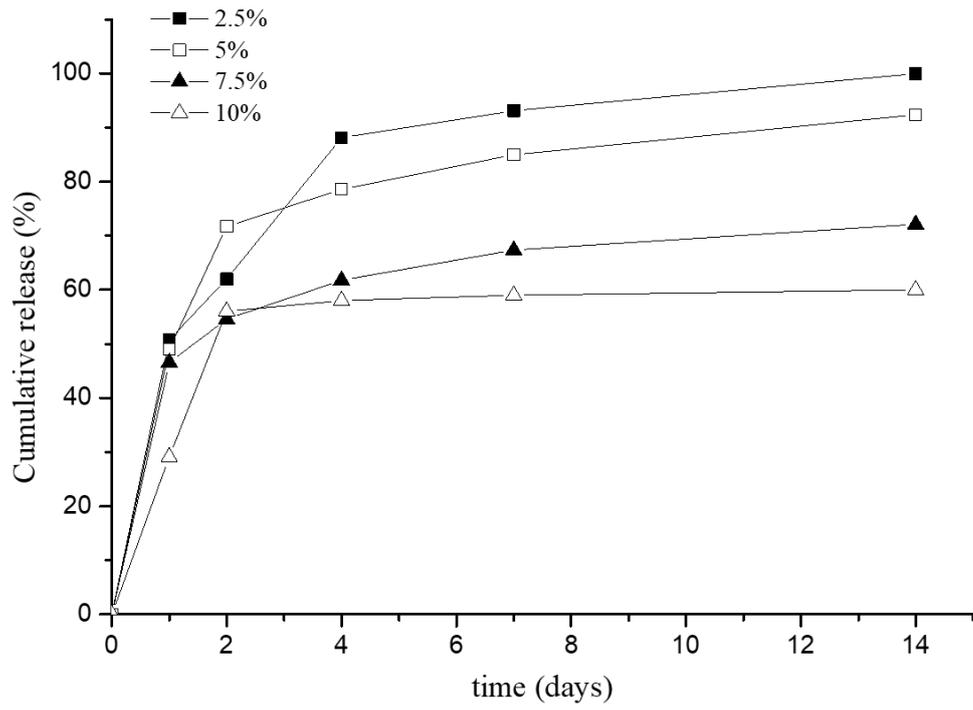
Grand Ballroom, THU 11:00~12:30

Biodegradable Double-Emulsion Nanoparticles Based on Polyfumarateurethane for Sustained Release of Bupivacaine

Soo Yong Park, Ildoo Chung*

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

Biodegradable polyfumarateurethane (PFU) for delivery vehicle using di-(2-hydroxypropyl fumarate) (DHPPF), PEG (polyethylene glycol) and HMDI (1,6-hexamethylene diisocyanate) was designed to be degraded through hydrolysis and enzymatic degradation mechanisms due to its ester bond along the polymer backbone. mPEG-PLA block copolymer was also synthesized by anionic ring opening polymerization of L-lactide onto mPEG (methoxy polyethylene glycol) to use for letting the interfacial layer stable. Using water-in-oil-in-water double emulsion technique, nanoparticles encapsulating water or fluorescein isothiocyanate were fabricated. The nanoparticles have PEG on their surfaces which helps nanoparticles to avoid the immune system. The morphology of these nanoparticles was characterized by DLS, TEM, FE-SEM and fluorescent microscopy. Encapsulation efficiency and in vitro drug release efficiency were also confirmed by UV/Vis spectroscopy.



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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Photocontrolled Cationic RAFT Polymerization of Vinyl Ethers

Chungsoo Kim, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

In this presentation, we provide our recent studies on the cationic RAFT (reversible addition-fragmentation chain transfer) polymerization of vinyl ethers using a combination of new organic photo-oxidants, chain-transfer agents (CTA), and visible-light irradiation. Variation of the photo-oxidant structures affected the absorbance profile in the UV-Vis absorption spectrum. Using this polymerization process, poly(vinyl ether)s with narrow molecular weight distribution were produced in the presence of a proper light source.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

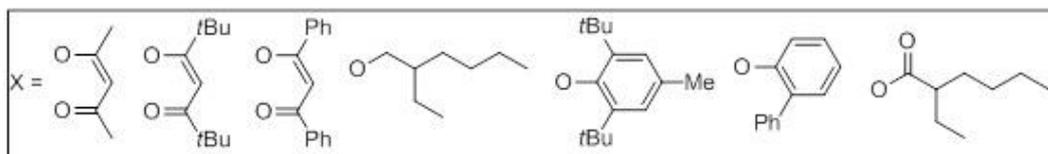
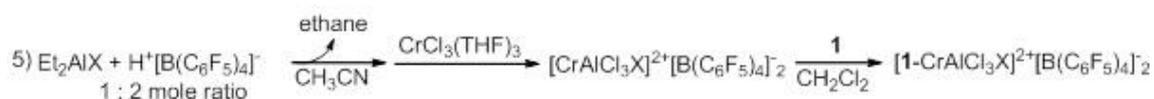
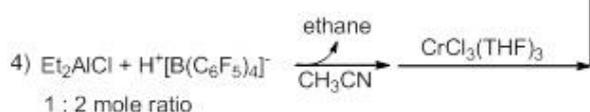
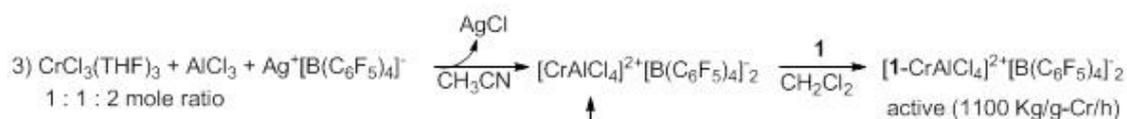
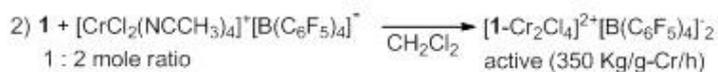
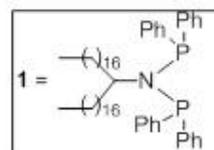
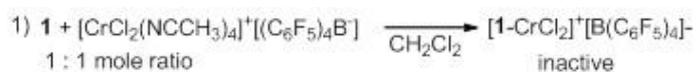
MAO Free and Extremely Active Chromium Catalytic System for Ethylene Tetramerization For Ligand Tuning

Hee soo Park, Bun Yeoul Lee*, Seung Hyeon Moon, Kyunglee Park

Department of Molecular Science and Technology, Ajou University, Korea

Ethylene tetramerization catalyst systems discovered by Sasol consist of Cr(III) source ($\text{Cr}(\text{acac})_3$ or CrCl_3), PNP ligand ($\text{RN}(\text{PPh}_2)_2$), and MAO are useful for the production of 1-octene through selective ethylene oligomerization.¹ When it comes to the large scale use of the Sasol system, The use of MAO in excess has economic burden because of expensive price of MAO. In this work, we developed a catalytic system using inexpensive alkylaluminum in place of MAO. $[(\text{CH}_3\text{CN})_4\text{CrIII}(\text{Cl}_2)]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ isolated in the reaction of $\text{CrCl}_3(\text{THF})_3$ with $[(\text{CH}_3\text{CN})_4\text{Ag}]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ is reacted with $i\text{PrN}(\text{PPh}_2)_2$ (1) or $[\text{CH}_3(\text{CH}_2)_{16}]_2\text{CHN}(\text{PPh}_2)_2$ (2) to produce cationic chromiumIII species bearing $\text{B}(\text{C}_6\text{F}_5)_4^-$ anion ($[\{i\text{PrN}(\text{PPh}_2)_2\}\text{CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ or $[\{\text{CH}_3(\text{CH}_2)_{16}\}_2\text{CHN}(\text{PPh}_2)_2\}\text{CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$). The molecular structures of $[(\text{THF})_4\text{CrIII}(\text{Cl}_2)]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ and $[1\text{-CrCl}_2(\text{THF})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ were unambiguously determined by X-ray crystallography. The cationic (PNP)CrIII complexes paired with $[\text{B}(\text{C}_6\text{F}_5)_4]^-$ anions, i.e., $[(\text{PNP})\text{CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ exhibited high activity with satisfactory selectivity when activated with common trialkylaluminum species (Me_3Al , Et_3Al , and $i\text{Bu}_3\text{Al}$) in chlorobenzene. Compared to original Sasol system ($(i\text{PrN}(\text{PPh}_2)_2)\text{CrCl}_3/\text{MAO}$ (200 Kg/g-Cr/h; 1-hexene 46%, 1-octene 40%, PE 1.2%)), These activity and selectivity are acceptable. When activated with Et_3Al or $i\text{Bu}_3\text{Al}$, the Cr complex $[2\text{-CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$, which bears long alkyl chains, showed high activity in the more desirable methylcyclohexane solvent (89 Kg/g-Cr/h) and much higher activity in cyclohexene (168 Kg/g-Cr/h). Other advantages of the $[2\text{-CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-/\text{Et}_3\text{Al}$ system in cyclohexene were negligible amount of side product (polyethylene, 0.3%), generation of fewer unwanted side products above C10, and negligible catalyst deactivation. The $[\text{B}(\text{C}_6\text{F}_5)_4]^-$ anion is compatible with trialkylaluminum species once it is not paired with a trityl cation. Therefore, $[(\text{PNP})\text{CrCl}_2(\text{CH}_3\text{CN})_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-/\text{Et}_3\text{Al}$ exhibited considerably higher activity than that of a previously reported system consist of $[\text{Ph}_3\text{C}]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$, i.e., $1/\text{CrCl}_3(\text{THF})_3/[\text{Ph}_3\text{C}]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-/\text{Et}_3\text{Al}$. Scheme 1 (or Figure 1).

Reference[1] M.J. Overett, K. Blann, A. Bollmann, J.T. Dixon, D. Haasbroek, E. Killian, H. Maumela, D.S. McGuinness, D.H. Morgan, Mechanistic Investigations of the Ethylene Tetramerisation Reaction, Journal of the American Chemical Society, 127 (2005) 10723-10730.



Poster Presentation : POLY.P-11

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

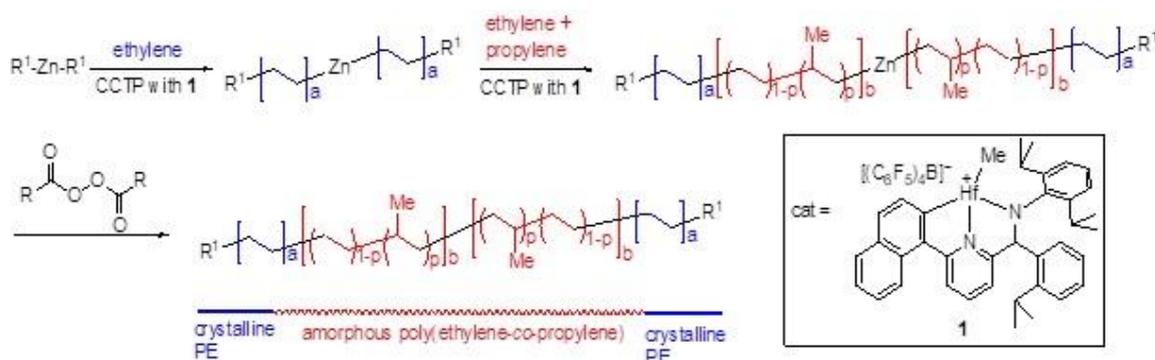
Preparation of ABA-type Olefin Triblock Copolymers based on Peroxide-Mediated Alkyl-Alkyl Coupling reaction

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In this study, a practical and simple method for the preparation of ABA-type olefin triblock copolymers, e.g., PE-b-poly(ethylene-co-propylene)-b-PE has been described. The performance of the so-called "coordinative chain transfer polymerization" (CCTP) by sequential feed of ethylene and ethylene/propylene mixed gas generated a Zn-bound diblock copolymer (i.e., (PE-b-poly(ethylene-co-propylene)yl)₂Zn). Treatment of the Zn-bound diblock copolymer with lauroyl peroxide (CH₃(CH₂)₁₀C(O)OOC(O)(CH₂)₁₀CH₃) lead to a C(sp³)-C(sp³) coupling reaction between the two diblock chains(PE-b-poly(ethylene-co-propylene)) bound on the zinc site and an ABA-type olefin triblock copolymer, PE-b-poly(ethylene-co-propylene)-b-PE, was formed. Upon the treatment with lauroyl peroxide, the number average molecular weight increased by 1.5–1.7 times. The occurrence of the coupling reaction was verified using a model compound, [(Oct)]₂Zn. The ABA-type triblock copolymer exhibited thermoplastic elastomeric properties and dramatically improved mechanical properties (twice the tensile strength and ten-fold increase in the elongation at break) as compared to the diblock congener.



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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Size-controlled Synthesis of Hyperbranched Polymer Nanoparticles

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Polymer nanoparticles have been used for a wide range of practical applications and their fundamental properties depend on the size of particles. In this study, the preparation of monodisperse hyperbranched polymer nanoparticles (HB-PNPs) in the different size range was explored by controlling the feeding rate and volume of monomer solution. The size, shape and surface properties of the resulting HB-PNPs were characterized by dynamic light scattering (DLS), FE-SEM and zeta potential measurements.

Poster Presentation : **POLY.P-13**

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Intramolecular Segregation In Heteroarm Core Cross-Linked Star Polymers

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Korea*

A heteroarm core cross-linked star (CCS) polymer is a subset of star polymers where two different polymer arms are covalently joined to a densely cross-linked core. Because the covalent connectivity prevents rearrangement of the polymer arms, it has been speculated that intramolecular segregation of the different polymer arms within the heteroarm CCS polymer would be difficult. Here we will explore how synthetic routes to the heteroarm CCS polymer influences on the intramolecular segregation behavior. We will monitor solution and bulk behaviors of heteroarm CCS polymers synthesized via different routes including “in-out” and “multimacroinitiator” methods, and rationalize the differences in terms of degree of intramolecular segregation.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Development of eco-friendly TPEE manufacturing technology

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Thermoplastic polyether ester elastomer(TPEEs) consist of two types of chemically different segments, hard-crystalline and soft-amorphous segments, and show a phase-separated microstructure. Due to the phase-separated microstructure, TPEEs combine the elasticity and flexibility of rubbers and the processability of thermoplastics. The properties of TPEEs depend on the chemical nature and incompatibility of the two types of segments, hard and soft, as well as on their mass ratio and respective lengths. Several kinds of monomers are used depending on the physical properties. Recently, as the interest in the environment has increased, we have developed a manufacturing method that can easily adjust the melting point while improving the environmental friendliness by using monomers derived from plant raw materials and maintaining the physical properties of TPEEs.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Thermoplastic polyether ester elastomer (TPEE) comprising environmentally-friendly Isosorbide derivatives and method of manufacture

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The thermoplastic elastomer having a hard segment and a soft segment is a polymer having both of a thermoplastic property that can be reformed upon heating and an elastic property of an elastomer that is a rubber-like polymer. Recently, it has been used in industrial fields for many purposes such as packaging containers, automobile interior materials, and elastic fibers, and the demand for it has been greatly increased because it is easy to recycle. In this study, we propose a thermoplastic polyether ester elastomer (TPEE) which can improve the environmental friendliness by incorporating the Isosorbide derivatives from biomass in the soft segment and can easily control the melting point while maintaining the elastic and physical properties of the thermoplastic elastomer.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Polybutadienes containing Triazoles via Click Reaction

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Hydroxy-terminated polybutadiene is widely studied and most used prepolymer for binder system of composite solid propellants, but it brings down the overall energy because of its inert nature. Polybutadienes containing triazole (PBT) overcome this limitation by introducing energetic groups into PB, so they can act as energetic binder. Furthermore, it is noteworthy that pendant functional group connected to triazole can be applied to further transformation of PBT. We prepared several phenyl-terminated polybutadienes (PtPBs) containing various triazoles via click reaction between azidated PtPB and alkyne derivatives. All of azide groups in polymer converted to triazolyl groups completely with high yield, and products were confirmed by NMR, IR, GPC and DSC.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Structure-controllable synthesis method that ladder structure and cage structure of polysilsesquioxane via the sol-gel reaction of various silane

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Polysilsesquioxanes were prepared by hydrolysis and condensation polymerization using various tri-functional alkoxide silane having a T₃ structure. Polysilsesquioxanes include three structures: random structure, ladder structure and cage structure. In this study, polysilsesquioxanes of cage structure and ladder structure were prepared at room temperature pressure by controlling silane concentration and amount of water in hydrolysis and condensation of various silane. Two types of products were analyzed by ²⁹Si-NMR to observe the T² and T³ peaks. The crystal lattice of products was confirmed by XRD analysis and a molecular weight of prepared products was compared with the predicted molecular weight of PSSQ's structure by MALDI-TOF and GPC analysis. A distinguishable synthesis of cage and ladder structures was observed by controlling the amount of water and silane concentration used for synthesis of polysilsesquioxane. The amount of water and concentration of silane are expected to determine the mechanism that the cyclic and linear compounds are synthesized.

Poster Presentation : **POLY.P-18**

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

A simulation study on the glass transition of polymer fibers with nanoparticles

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Polymer fibers have been used in various applications (including energy storage and electronic devices) due to excellent thermal and mechanical properties, especially the glass transition temperature (T_g). Previous experiments revealed that the addition of nanoparticles (NPs) into polymer fibers could control T_g of polymer fibers. The glass transition temperature of polymer fibers, however, is yet to be understood at the molecular level. For example, there has been a controversy over the effects of the addition of NPs on the glass transition temperature. T_g of polymer fibers increases for some NP types, whereas T_g of polymer fibers decreases for other NP types. In this work, we perform molecular dynamics simulations for polymer fibers with NPs of different types of intermolecular interactions and investigate the glass transition and dynamics of polymer fibers. We prepare polymer fibers without NPs and with NPs of different interaction types. We illustrate that, upon the addition of NPs, T_g of polymer fibers depends on the interaction types of NPs. Adding NPs with attractive interactions increases T_g of polymer fibers, whereas adding NPs with relatively repulsive interactions decreases T_g of polymer fibers. We also find that the interaction types of NPs affect the mobility of monomers not only near NPs but also out of interaction ranges of NPs: when the interaction type of NPs is attractive (repulsive), the mobility of monomers decreases (increases). Such effects of NPs on the dynamics of polymer fibers cause the changes of T_g .

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Improvement of the diffraction efficiency of a polymer by using various Ionic Liquids

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In our studies, different kinds of photosensitive materials for information storage devices have been studied. We synthesized the polymer through the surface relief grating (SRG) fabrication with a diode-pumped solid-state laser (DPSS) of 532 nm. As a result of the measurement of the diffraction efficiency (*DE*) of the polymer synthesized by using a low power DPSS laser at 633 nm, a low diffraction efficiency was obtained, even after 15 min of exposure. In order to solve this problem and reduce the *DE* measurements time, we tried to introduce various ionic liquids (ILs) at the polymer. Through various ILs such as imidazolium ILs and ammonium ILs, We have investigated the *DE* and the measurement time of the polymer with ionic liquids, as a result, it was confirmed that the polymer with ionic liquids showed better results. These studies have not been conducted with azo-polymer and IL mixture in past. Hence, these results seem to be beneficial in the field of polymer chemistry and holographic research.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Large size PbS quantum dot solar cells with IR absorption

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Today, there has been a growing interest in solar cells capable of absorbing the infrared(IR) region. IR-absorbing photovoltaics can improve the limitation of visible-absorbing photovoltaics with tandem structure. However, high performance IR solar cells can only be made of wafer type inorganic, which has high cost materials and fabrication method problem. In case of inorganics, the stability is main issue. The quantum dot is good alternative for IR-absorbing photovoltaics, because it has controllable band gap and high optoelectronic properties with ligand passivation. The problem is that it is hard to apply the inorganic halogen ink ligand exchange directly because quantum dots show different surface properties as there size with different grown surface. Using our new exchange method, we have fabricated well-passivated large size quantum dot and solar cells. The filter lens was used to check the absorption over ~800 nm.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

A Series of Novel Conjugated Polymers Based on Fluorene and Fluorinated Quinoxaline for OPVs

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¹Engineering Chemistry, Pukyong National University, Korea

The novel copolymers using fluorene and fluorinated quinoxaline were synthesized by Suzuki and Stille coupling reactions. The polymers had good solubility in organic solvent such as benzene derivative (toluene, chlorobenzene and o-dichlorobenzene). The absorption spectra in solution had maximum peak at 442 to 498 nm and in solid film had maximum peaks at 448 to 543 nm. These polymer have improved π - π interchain interactions in the film state compared to those in solution. These polymer observed a narrow bandgap 1.93 to 2.14 eV. A highest occupied molecular orbital (HOMO) energy level showed at -5.59 to -5.67 eV and lowest unoccupied molecular orbital (LUMO) energy of -3.51 to -3.72 eV. PSCs made from copolymer:PC70BM (1:1.5 wt%) + 3vol% DIO blends showed maximum power conversion efficiencies (PCE) values of (3.98, 2.91, 3.33, 3.55 and 3.07%), respectively.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Characterization of Self-Polishing Polyurethane Copolymers

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One of effective strategies in self polishing industries is containing a zinc acrylate monomers. In this work, we synthesized and designed self-polishing polyurethane copolymers to enhance their adhesion to the surface. Synthesized polyurethane based copolymers were investigated by Fourier transform infrared (FT-IR) and inductively coupled plasma optical emission spectrometry (ICP-OES). The properties of polyurethane based copolymers containing Zn were compared with the zinc-free polyurethane as reference. The polishing rate was determined by measuring the film thickness after dynamic immersion tests. Compared with the zinc-free polyurethane, the experimental results demonstrate that polyurethane based self-polishing copolymers show good self-polishing properties and adhesion to the surface.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Comparison of New Small Molecular based on Benzodithiophene and Fluorinated-Quinoxaline According to Alkyl Side Chain

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The small molecular (EH-BDT(DTDFDDoQx)₂, EH-BDT(DTDFDHexQx)₂, Oct-BDT(DTDFDDoQx)₂, and Oct-BDT(DTDFDHexQx)₂) were synthesized by stille coupling reaction. These small molecular showed similar λ_{max} in solution (475, 471, 475 and 468nm) and in film (538, 536, 538 and 540nm) state. And similarly other series, bathochromic shift was taken in film state (about 65 nm ~70nm). The benzodithiophene (BDT) unit was used as electron rich unit and quinoxaline (Qx) unit was used as electron poor unit to make donor-acceptor type small molecular solar cells. According to alkyl length of benzodithiophene and quinoxaline, the characteristics of organic solar cells were compared. These small molecular had same backbone except for alkyl side chain, so this series indicated similar electrochemical properties. A highest occupied molecular orbital (HOMO) energy level showed (-5.27 to -5.38 eV) and lowest unoccupied molecular orbital (LUMO) energy level (-3.17 to -3.21 eV) respectively. Under optimized states, the efficiency of (EH-BDT(DTDFDDoQx)₂ was achieved 1.20% of power conversion efficiencies (PCE).

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Effects of the addition of the NaOH-containing functional aliphatic compounds on the aggregation behavior of asphaltenes in a heavy oil

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In this work, we studied the effects of the addition of mixtures of NaOH and functional aliphatic compounds on the dispersion of asphaltenes in a heavy oil. In this work, the functional groups of the organic compounds were alcohol, amine, and carboxylic acid. It was found that either NaOH or each organic compound did not show improved dispersion behavior of the asphaltenes by the addition of itself to the oil. However, when NaOH was mixed with the functional compounds, the mixture enhanced the dispersion of the asphaltenes in the oil. In addition, it was observed that the effects of the addition of NaOH-containing dispersant on the dispersion of the asphaltenes became stronger in the following order: the amine dispersant < carboxylic acid dispersant < alcohol dispersant. Furthermore, it was found that when the organic compound had a side chain, its dispersion property was improved. Thus, we proposed that NaOH-containing branched aliphatic compounds could be used as effective dispersants for the asphaltene in a heavy oil.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Comparative Study of a Variety of Hetero Aromatic Oligomers

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We have studied various conjugated hetero aromatic oligomers that is synthesized to make conjugated polymers. Conjugated polymers have been used as active layers for various kinds of conductive device application. Conjugated oligomers with electron donor-acceptor structure have also low band gap and these properties can be applied for a wide range of conductive polymers. In this work, we compared several types of oligomers synthesized in our laboratory. The structure of the compounds was identified by ¹H NMR, ¹³C NMR, and FT-IR spectroscopy. We also posted each UV-vis absorption, photoluminescence(PL) spectra for the synthesized compounds. Through this work, we can check the efficiency of each oligomers and it is expected to be applied to the photovoltaic devices, organic solar cell, organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), and electrochromic devices, etc.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Effect of Interaction between the Newly Synthesized Conducting Polymer and Ionic Liquid on Physical Properties

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In this study, we synthesized a new thiophene-based conducting polymer, 2-heptadecyl-5-hexyl-6-(5-methylthiophen-2-yl)-4-(5-((E)-prop-1-enyl)thiophen-2-yl)-5H-pyrrolo[3,4-d]thiazole (HHMPT). To increase its application, the interactions between the conducting polymer (HHMPT) and ionic liquids (ILs) were investigated by UV-Vis spectroscopy, FTIR spectroscopy, and confocal Raman spectroscopy techniques. Additionally, film roughness and conductivity of the polymer film with or without ILs were studied. As a result, this study revealed that the imidazolium family IL-polymer mixtures and ammonium family IL-polymer mixtures have almost similar conductivity at low concentration of ILs. Also, this study provides an insight into the combined effect of a polymer and ILs and may generate many theoretical and experimental opportunities.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation and Physicochemical Characterization of Magnetic Agarose Beads for Protein Purification

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Agarose beads have been studied for efficient separation and purification of tagged specific proteins. In this study, agarose beads having magnetic iron oxide particles were prepared by using emulsion droplet gelation method and their physicochemical characteristics were studied. Black Fe₃O₄ particles were prepared by co-precipitation of Fe(II) and Fe(III) ions with an alkaline solution. Agarose aqueous droplets having Fe₃O₄ particles were formed in a water-in-oil emulsion prepared by emulsification of the hot agarose aqueous solution in an organic solvent such as cyclohexane. Gelation of agarose by cooling of the droplets gave magnetic agarose beads. An average size of the beads prepared at fairly optimized conditions was 100 micrometers. The Fe₃O₄ contents in agarose beads were determined by an inductively coupled plasma analysis. Crystalline peaks of Fe₃O₄ particles and changes of the peaks of magnetic agarose beads were identified by X-ray diffraction analyses. To strengthen magnetic agarose beads, the agarose was crosslinked with epichlorohydrin. Physicochemical properties of the crosslinked magnetic beads were characterized by swelling ratio measurement and FT-IR, TGA, DSC analyses etc.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Structure-Property Relationships in Quinoidal Conjugated Polymers Containing Different Length of Core

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Conjugated molecules containing quinoid structures have been extensively studied as organic electronics requiring efficient charge transport due to their high structural planarity arising from a double bond linkage between aromatic rings. Their planar structures induce a favorable π -electron delocalization over the whole backbone as well as an efficient intermolecular π -orbitals overlap; thereby, they manifested very promising charge transport properties. However, quinoid compounds have been rarely used as the building block for conjugated polymers. To achieve the incorporation of quinoidal platform into the polymer backbones, we have utilized an isatin unit which has bromine at 6-position possible to polymerization. Recently, we have reported quinoidal conjugated polymers incorporating an isatin-terminated quinoid units, quinoidal thiophene (QuT), with common aromatic rings. These polymers are applied to organic field-effect transistors as an active layer, and they showed high mobility over 2 cm²/Vs. In this research, we investigate the change of properties in accordance with the length the quinoid unit in the polymer backbone. Two quinoid monomers, QuT and quinoidal bithiophene (QuBT), were synthesized simultaneously via one-pot reaction. Then, two quinoid polymers based on these units, poly(quinoidal thiophene-thienylene vinylene) (PQuT-TV) and poly(quinoidal bithiophene-thienylene vinylene) (PQuBT-TV), were developed by copolymerization with a thienylene vinylene which has an extended conjugation. We discuss the correlation between the molecular structures and the various properties of these polymers.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation and Polymerization of Ophthalmic Lens containing Anisole Group

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The characteristics of anisole group and hydrogel monomers by ratio in order to check their commerciality and their utilization as additives were investigated. The 2-hydroxy ethyl methacrylate(HEMA), Ethylene glycol dimethacrylate(EGDMA), Methyl methacrylate(MMA) and Methacrylic acid(MA) were basic unions, Azobisisobutyronitrile (AIBN) was used as an initiator. In addition, the additives 2-, 3- and 4-Methylanisole were added at 1 to 10% ratio to combine them with thermal polymerization. After measuring the refractive index, water content, and spectral transmittance rate of each specimen manufactured, the results were compared and analyzed in proportion. As a result of measurement of the manufactured contact lens, the refractive index of the 2MET sample was 1.4169 ~ 1.4221, the water content was 44.71 ~ 45.92%, and the spectral transmittance in the visible light range was 90.87 ~ 91.14%. The 3-MET sample has a refractive index of 1.4216 ~ 1.4249, a water content of 40.96 ~ 43.99 and spectral transmittance of 90.26 ~ 93.72% in visible light region. The 4-MET sample has a refractive index of 1.4064 ~ 1.4205, a water content of 44.34 ~ 45.73%, and a Spectral transmittance of 94.06 ~ 92.79% in visible light region. In case of 4-MET sample, the water content decreased as the proportion of additives increased, while the 2-MET and 3-MET increased. In particular, The 2-MET sample has a much higher water content than 3-MET and 4-MET in the same proportions, thus it can be used as a material for high-functional contact lenses.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

UV-blocking and High Oxygen Permeable Ophthalmic Lens Containing benzophenone and benzotriazole Group with Oxide Nanoparticles

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To minimize the ophthalmic side effects caused by corneal hypoxia and UV light, the functional silicon hydrogel ophthalmic lens containing UV absorbents and oxide nanoparticles were manufactured. 2H4O (2-Hydroxy-4-n-octyloxybenzophenone) and 25CB (2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chloro-2H-benzotriazole) as UV-blocking material and oxide nanoparticles were used as additives with silicon monomers. The materials were copolymerized with EGDMA (ethylene glycol dimethacrylate) as the cross-linking agent and AIBN as the initiator. Measurement of the physical characteristics of the produced material showed that the refractive index is 1.3822~1.3957, water content 60.33~62.95%, UV-B transmittance 0.12~57.29%, UV-A transmittance 0.02~83.15% and DK 20.84~33.05 $\times 10^{-11}$ (cm²/sec)(ml O₂/ml \times mmHg). The polymer including silicon monomer showed high performance of oxygen permeability and water content. Also, the results showed increase of UV-blocking effect as the ratio of additives and copolymerization of both absorbent and nanoparticle made synergy effect of UV-blocking. Based on the results of this study, the transmittance for UV was reduced significantly with increase of 2H4O, 25CB and oxide nanoparticles. These materials are expected to be used as useful material for UV-block ophthalmic lens with high water content and oxygen permeability.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Comparison of PNIPAM hydrogels synthesized by γ -ray radiation and chemical method

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The mechanical and chemical properties of poly(n-isopropylacrylamide) hydrogels were investigated. Three different methods were used preparing PNIPAM hydrogels; one is synthesized by γ -ray irradiation to the monomer-clay solution (direct method), another is by γ -ray irradiation to the clay solution to get radical itself (indirect method) and the other is by potassium persulfate (KPS) initiator (chemical method). γ -ray generates radicals in the solution and forms 3D network without any crosslinker while the chemical method use KPS as a crosslinker. The saturation ratio and the time of swelling were investigated, and the structural changes during swelling were measured by the following techniques; rheometer, Fourier-transform infrared spectroscopy (FTIR) and small-angle X-ray scattering (SAXS). Among these three methods, only chemical method showed self-healing property. Furthermore, it showed the best swelling property because of the structural difference. The morphology of PNIPAM hydrogel was also investigated to see microscopic structural changes using scanning electron microscope (SEM).

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Click reaction-derived supramolecular nanoreactors based on aqueous assembly of amphiphilic molecules

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¹School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea

A water-processable nanoreactors are increasingly investigated to develop the environment-friendly catalyst. Amphiphilic molecules can self-assemble into various nanostructures such as micelles, fibrils, vesicular structures and sheets, etc depending on the molecular design. Especially, supramolecular nanoreactors based on amphiphilic molecules are of great interest as a nanocatalysts with large quantity of catalytically active sites within the nano-architectures. Meanwhile, "click chemistry" has been widely used to prepare new functional materials by allowing to link together different molecular fragments with synthetic simplicity, mild reaction condition, fast and quantitative reaction. Interestingly, the resulting click-derived triazole group plays a role as a ligand for chelating metal ion with specific binding affinity depending on the triazole-containing molecular structure. In this work, triazole-based amphiphilic molecules containing aromatic and hydrophilic tri(ethylene oxide) segment were easily synthesized using facile click chemistry. The Cu²⁺-nanoassemblies can be a facile nanocatalyst for activating the azide-alkyne cycloaddition in aqueous medium by reduction of the Cu²⁺ to Cu⁺. The interesting point is that the metal-captured nanostructures can induce the molecular synthesis by click reaction in water and further, the click-derived products could control the morphology of nanoreactor depending on the molecular structure of products.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and characterization of PNiPAAm-based copolymer

Yeonju Park^{*}, Young Mee Jung^{*}

Department of Chemistry, Kangwon National University, Korea

Poly(*n*-isopropylacrylamide) (PNiPAAm) is one of the stimuli-responsive polymer, which respond to temperature. PNiPAAm has lower critical solution temperature (LCST) at 32-34 °C, which is near the normal human body temperature. Therefore, it has been used for many fields in sensing, drug delivery, tissue engineering, and so on. However their application has been limited because of their relatively slow responds time to solution pH changes, toxicity, and very stable to decomposition. To overcome this problem, PNiPAAm-based copolymer has been synthesized by many researchers. In this study, we synthesized the poly(NiPAAm-*co*-acrylic acid) (PNiPAAm-*co*-AA) polymer and characterized it using infrared spectroscopy. The details of this study will be discussed in this presentation.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Development of cyclic olefin copolymer-based immunoassay chips using functional polymer

Daekyung Sung

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Korea*

We developed cyclic olefin copolymer-based immunoassay chips through pre-activated polymer adlayers. For the surface modification of COC substrates we synthesized two types of amphiphilic polymers having three important functions: hydrophobic groups, a PEG component, and an NHS ester group for conjugation of biomolecules. Formation of the polymer adlayers on COC surface was confirmed using a contact angle analyzer. Sandwich immunoassay using anti-rabbit IgG immobilized COC surface showed linear response to rabbit IgG of model analyte over a range from 1 to 1000 ng/mL with detection limit of 1–10 ng/mL. We also fabricated a Lab-On-a Chip type of COC biochip, which could detect a cardiac marker protein, troponin I (TnI), with detection limit of 10 ng/mL.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation and thermomechanical properties of thermoset polyurethane shape memory polymers

Jamin Gu

R&D Center, NOROO Paint, Korea

This study is to investigate the thermomechanical properties according to the change of hard and soft segment ratios and diol types of polyurethane-based thermoset shape memory polymers(SMPs). SMP films were prepared by reaction of IPDI-prepolymer and three-functional polycaprolactone(PCL) diol. The three kinds of IPDI-prepolymers were synthesized with three different diols that were bisphenol-A, polyoxyethylene bisphenol-A ether and polytetramethylene ether glycol(PTMEG). Also, each IPDI-prepolymer was designed to have different isocyanate equivalent weight. the glass-transition temperature was characterized by dynamic mechanical analysis(DMA), fixity and recovery ratios are investigated using universal testing machine(UTM).

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Internal structure and optical property of end-crosslinked poly(ethylene glycol) network

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Neutron Science Center, Korea Atomic Energy Research Institute, Korea

¹Department of Chemistry, Hanyang University, Korea

This study reveals the internal structure of poly(ethylene glycol) (PEG) network with chain ends crosslinks. PEG networks with different molecular weight and volume fraction were observed by using small-angle neutron scattering and X-ray scattering. The networks exhibited certain domains determined by molecular weight between crosslinks. The overall inhomogeneities of the gels were influenced by volume fraction. The occupation of local domains, consisting of entangled chains or lamellar stacks, were proved from the swollen and cast networks. The results demonstrate the optical properties caused by the localized polymer density in the network, and they provide the ideas to prepare contraollable network architecture.

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

Polymer Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Properties of 1,3,5-Triazine based Tri-functional Epoxy Resin

Miyeon Lee, Jong-jin Park¹, Munju Goh^{2,*}

Korea Institute of Science and Technology, Korea

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²*Institute of Advanced Composite Materials, Korea Institute of Science and Technology, Korea*

Epoxy resins have been industrially adapted as matrix for composites due to their excellent properties such as adhesiveness, heat resistance, and chemical resistance. In recent years, along with the increasing usage of high-performance composite materials, the industrial needs for the high-performance epoxy resins also steadily increases. Conventional methods for obtaining high strength and high heat resistance performance have been widely used for increasing the number of epoxy groups in a molecule. It is also required to develop epoxy resins having molecular symmetry so as to be advantageous for compounding with various filler materials. To this end, we synthesized tri-functional epoxy resin bearing 1,3,5-triazine core with C3 symmetry. We will discuss more detailed synthetic methods and thermal and physical properties of epoxy resin.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Home built double resonance probes for non-spinning Solids NMR

Ji-Ho Jeong, Ji Sun Kim , Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Solid state NMR has seen a constant increase in popularity since the NMR had been first invented because it hurdled the biggest problem; inherent lack of resolution relative to solution state NMR; with many techniques. Solid state NMR serves many insights for organic and inorganic chemistry, where is used as a powerful tool to study local dynamics, kinetics as well as thermodynamics of a variety of systems. The assemblies of the NMR spectroscopy are magnet, computer, console and the probe. Of course, many factors of each assembly determine the performance of the NMR spectroscopy. Especially, the probe is the interface between a sample and the spectrometer. Its high solidity and flexibility are very important elements for supporting the maximum performances of the NMR spectrometer. Above all, the choice of probe suitable for various types of samples is needed for getting right results from NMR experiments. So we made the elaborate solid-state NMR probes for diverse sample analysis such as characterizing membrane proteins and defining of molecular dynamics in high tech devices. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) & narrow bore (NB) ¹H-¹⁵N solid-state NMR probe and a home-built 800 MHz NB ¹H-¹⁵N solid-state NMR probe for lossy samples. We will also announce a home-built 400MHz and 500 MHz NB ¹⁹F-¹³C solid-state NMR probes for analyzing nano-materials and LCD panel respectively and 600 MHz NB ¹⁹F-⁷Li solid-state NMR probes with solenoidal coil for investigating Li-ion battery. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. And finally we will introduce our recent commission task project “Development of sample dependent Solid-state NMR probe for the analysis of nanomaterials”.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Friction reducing effect of HRPB350 derivatives

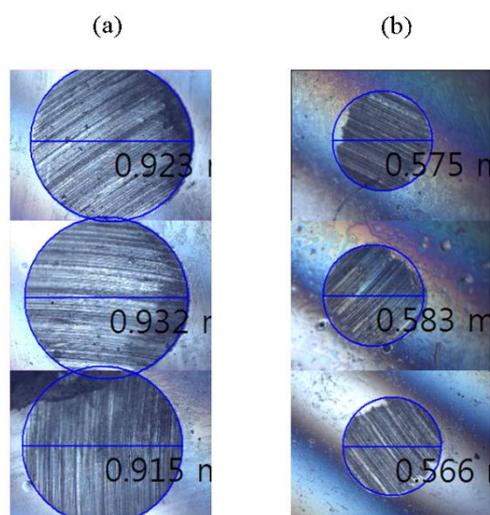
Min Sup Park, Joonho Kim¹, Yeong-Joon Kim^{1,*}, Jaehye Song²

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HRPB350 (highly reactive polyisobutylene, m.w.=350) derivatives were synthesized by the reaction of some compounds having S and N atoms and HRPB350. These are widely used as lubricant additives and fuel detergents. In order to study the friction reducing effect of these derivatives, we measured the size of the 4-ball WSD(wear scar diameter). The 4-ball WSD was significantly reduced when the HRPB350 derivatives was added in base oil compared to the case without additives. It was also confirmed that friction reducing effect of these derivatives was similar to that of the industrial products. Micrographs of worn scar when lubricating (a) without, and (b) with 1% of an HRPB350 derivative in base oil at the load of 392 N and 1 hour



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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of polybutylene derivatives having an N and S heterocyclic moiety

Joonho Kim, Min Sup Park¹, Yeong-Joon Kim*

Department of Chemistry, Chungnam National University, Korea

¹SCT, Daelim Industrial Co., Ltd, Korea

Introducing polar groups into highly reactive polybutylene is important because these types of derivatives could be used as fuel detergents, and lubricant additives. Highly reactive polybutylene (HRPB) with a vinylidene content of over 70% was obtained from the crude polybutylene mixture by vacuum distillation. In the first synthetic step, HRPB was reacted with maleic anhydride, Br₂, or HBr. Finally, HRPB derivatives were synthesized by the reaction with thiadiazol, thiazol, diamine, and so on. The final products were characterized by ¹H-NMR, ¹³C-NMR, and Mass spectrometry.

Poster Presentation : **IND.P-4**

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Facile synthesis of ultra-microporous carbons for selective CO₂ adsorption

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Microporous carbon materials are envisaged as efficient contenders for mitigating CO₂ levels by virtue of their favorable surface chemistry, high specific surface area, tunable pore structures, moderate heat of adsorption, and facile regeneration. This study presents a solvent-free one-step polymerization and activation method for designing a series of nitrogen-enriched carbons to delineate the role played by nitrogen moieties and ultra-micropores on CO₂ capture. The optimized material, MCKC-3, possesses high surface area (2060 m²/g) comprising of ultramicropores (

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Molten salt eutectic mixture: an effective medium to design microporous carbon-based adsorbents

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Microporous carbons with high specific surface area (around 3000 m²/g) were prepared by a single all-in-one route involving the simultaneous polymerization, carbonization and in situ activation of melamine and isophthalaldehyde mixture. It was revealed that carbon materials prepared at 700 °C, in the presence of KOH, exhibits a narrow pore-size distribution than those prepared in the presence of eutectic mixture. Additionally, MIK-700 possesses high micropore volume and as a result present an excellent CO₂ adsorption capacity of 9.7 mmol/g at 273 K and 1 bar. Similarly, the high specific area and pore volume contribute a major role in H₂ storage at 77 K, exhibiting 4.0 wt. % up take by MIKN-800 (2984 m²/g and 1.98 cm³/g specific surface area and pore volume, respectively).

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Nitrogen-doped highly porous carbons as a promising candidate in clean energy and environmental applications

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Microporous carbon materials are envisaged as efficient contenders for mitigating CO₂ level and global climate change by virtue of their rich surface chemistry, high specific surface area, tunable pore structures, moderate heat of adsorption, and facile regeneration. Current work presents a solvent-free one-step polymerization and activation approach for designing a series of microporous carbons using economically favorable avenue. Synthesized carbon materials possess a high surface area (1360-4288 m²/g), large pore volumes (1.15-3.04 cm³/g), and hierarchical meso-micro and ultramicroporous structures. The high adsorption capacities with the facile regeneration make these microporous carbons amongst the most promising adsorbents in clean energy and environmental applications.

Poster Presentation : **IND.P-7**

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

MnO₂ and biomass-derived 3D porous carbon composites electrodes for high performance supercapacitor applications

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

MnO₂/biomass-derived porous carbon (BPC) composites have been prepared by a hydrothermal method, in which the BPC 3D porous carbon structure was based on a banana peel. The banana peel, after freeze drying, can maintain its hierarchical natural porous structure, which provides enough growth space for MnO₂ and reduces the agglomeration of MnO₂ particles. The MnO₂/BPC composites were characterized by XRD, FT-IR, XPS, TGA, SEM, TEM, BET. The electrochemical performance of the composites was tested in three-electrode supercapacitors using 1 M Na₂SO₄ aqueous solution as an electrolyte. Due to the large amounts of hierarchical pores and large pore volume, the as-prepared composites exhibited good electrochemical performance. Electrochemical measurements indicated that the MnO₂/BPC composites applied in supercapacitors had a specific capacitance of 139.6 F g⁻¹ at 300 mA g⁻¹, and exhibited a good cycling stability with a capacitance retention ratio of 92.3% after 1000 cycles (at 1 A g⁻¹). The MnO₂/BPC composites with 3D porous structure are promising materials in the application of supercapacitors.

Poster Presentation : **IND.P-8**

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Facile hydrothermal synthesis of NiCo₂O₄- decorated filter carbon as electrodes for high performance asymmetric supercapacitors

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

A simple hydrothermal method is developed for the growth of NiCo₂O₄ nano-needle arrays on a filter paper carbon (FC) substrate for use as a high performance electrode for supercapacitors. The as-synthesized NiCo₂O₄/C composites exhibited high specific capacitance (995.2 F g⁻¹ at a current density of 10 A g⁻¹.) and excellent cycling performance (no capacitance loss after 3000 cycles). The 3D framework of the FC substrate not only prevents the aggregation of NiCo₂O₄ nanoparticles, but also improves its electrical conductivity, thus leading to excellent electrochemical performance. Moreover, an asymmetric supercapacitor was assembled by using the NiCo₂O₄/C composites and activated carbon as the positive and negative electrode, respectively, and provided a maximum energy density of 20.87 Wh kg⁻¹ at a power density of 374.6 W kg⁻¹ and a maximum power density of 7.48 kW kg⁻¹ at an energy density of 11.43 Wh kg⁻¹ within a potential window of 0-1.5 V, demonstrating the potential of the composites for use in high performance energy storage systems.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Photocatalytic hydrogenation of styrene in alcoholic suspensions of integrated NiWO₄/g-C₃N₄ nanocomposites in the absence of hydrogen gas

Kiran Naz, Soo-Jin Park^{1,*}

Inha University, Pakistan

¹*Department of Chemistry, Inha University, Korea*

By using reflux calcination method, facile fabrication of NiWO₄/g-C₃N₄ nanocomposites were accomplished. Upon purging with N₂, the as-prepared nanocomposites found an active visible-light-driven photo-catalyst for the hydrogenation of styrene to ethylbenzene in alcoholic suspension. Moreover, the hydrogenation intermediates were acknowledged by using gas chromatography–mass spectroscopy (GC-MS) and UV-Visible spectroscopy. This novel catalyst exhibited excellent catalytic activity and stability in styrene hydrogenation with no considerable loss of its initial activity for up to five times of recycling. At the same time, this method eliminated the use of high pressure hydrogenation reactors without the need for external sources of energy.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Photocatalytic hydrogenation using metal catalyst under visible light irradiation and their characterization

Kiran Naz, Soo-Jin Park^{1,*}

Inha University, Pakistan

¹*Department of Chemistry, Inha University, Korea*

Design and synthesis of low-cost photocatalyst with high activity and stability for hydrogenation reactions is an important research area of applied catalysis. Hydrogenation introduces structural defects, leads to disaggregation and fragmentation, and increases the specific surface area. Our study provide guidance for selective transformation of organics via construction of heterojunction photocatalysts. A wide range of applications can be expected for this efficient, and highly selective photocatalysis system in reduction reactions for the synthesis of fine chemicals.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Modified activated carbon supported with MnO₂ nanoparticles for lithium adsorption and recovery from aqueous solution

Urooj Kamran, Soo-Jin Park^{1,*}

CHEMISTRY, Inha University, Pakistan

¹Department of Chemistry, Inha University, Korea

Chemically treated activated carbon (CAC) decorated with manganese dioxide (MnO₂) was prepared using different Mn salt concentrations as a facile impregnation approach for enhancing the capacity of activated carbon for lithium adsorption. The morphological and physico-chemical properties were characterized. A batch experiment was performed to optimize the parameters (pH, adsorbent dose, and contact time) for Li⁺ adsorption. A kinetic study indicated that lithium sorption process followed a pseudo-second order reaction. Comparative analysis showed that adsorption capacity of the functionalized activated carbon with various manganese contents increased with an increase in manganese loading, CAC-Mn0.1, CAC-Mn0.12, CAC-Mn0.15, and CAC-Mn0.2, with values of 54%, 70%, 75%, and 96%, respectively. A desorption study was performed to make process more efficient. Overall, it is concluded that the synthesized nanocomposites can be effectively used in lithium adsorption and recovery from aqueous solution.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Reduced graphene oxide decorated with Ni-MnO₂ nanorods for lithium sorption and desorption from aqueous media

Urooj Kamran, Soo-Jin Park^{1,*}

Inha University, Pakistan

¹*Department of Chemistry, Inha University, Korea*

The weight ratios controllable synthesis of novel and effective RGO-Ni_x/MnO_{2y} nanocomposites was done by hydrothermal approach. The reduction of graphite to graphene oxide, fabrication of MnO₂ and deposition of Ni-MnO₂ above the surface of reduced graphene oxide was individually carried out by hydrothermal technique. The physical and morphological properties of prepared nanocomposites was analyzed. The batch adsorption experiment was performed to identify the lithium uptake capability of nanomaterials, in this study following parameters optimized to enhance adsorption rate; including effect of pH, dosage, contact time, and preliminary Li⁺ solution concentrations. The various kinetics and equilibrium isothermal models applied on experimental data to identify the nature of adsorption phenomena. To make process more economic and efficient, the Li⁺ desorption experiment performed. Briefly, it can be concluded that the prepared nanocomposites possessed adequate potential for lithium uptake.

Poster Presentation : **IND.P-13**

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

The Evaluation of the Preparation and Characterization of a Modified Carbon Black based on Specialty Carbon Black (SCB)

Dong Jun Park, Byung Min Lee, Soo Youl Park*

*Interface Material and Chemical Engineering Center, Korea Research Institute of Chemical Technology,
Korea*

The modified surface of specialty carbon black (SCB) is one of the main technical factors for producing a uniform color and stable dispersion. In this work, the carboxylation or sulfonation process of SCB was used to improve the dispersive properties of hydrophilic solvents such as 1,6-hexanediol and propylene glycol monomethyl ether acetate (PGMEA). The results showed that the color strength of SCB DC2500G changed little with a range of 0.128 ~ 0.941 (ΔE) compared to other SCB DC2500G material. In contrast, in the case of SCB EG410, there was a uniform color value with a range of 0.144 ~ 0.252 (ΔE). Also, in our experiments, a modified SCB was confirmed by printing ink material as a melt coating paper. It may be possible that the SCB EG410 material can be advantageous as a gravure ink product. Finally, the modified SCB obtained from this research will have a large impact on the industry as a potential material for toners, paint, rubber, fillers, and other carbon black additives.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

H₂O₂/steam activation as an eco-friendly and efficient topdown approach to enhancing porosity on carbonaceous materials for CO₂ capture

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In carbonaceous materials, physical activation by steam or carbon dioxide (CO₂) is a common top-down method that is known to be effective for developing nanopores on carbon surfaces. However, it is less efficient at improving porosity compared to common chemical activation. Here, we propose a simple and eco-friendly approach to improving the efficiency of physical activation in developing porosity on carbonaceous materials. Using hydrogen peroxide (H₂O₂) as an activating agent with pressure in the reactor resulted in significant enhancement compared with steam activation without pressure. However, a high number of oxygen functionalities were generated on the carbon surfaces, which interfered with CO₂ capture performance (e.g., uptake, selectivity, and the adsorption rate). We used thermal reduction to remove oxygen functionalities on the carbon surface, which overcame the CO₂ affinity and uptake loss caused by the oxygen functionalities. Therefore, H₂O₂/steam activation approach may be a way to improve the textural properties of carbonaceous materials. Furthermore, our work provides evidence that the oxygen functionalities of solid carbonaceous adsorbents influence CO₂ capture performance, including practical applications.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of highly porous carbon aerogels for hydrogen storage and supercapacitor applications

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, carbon aerogels (CAs) were prepared as physisorbents and electrode materials for hydrogen storage and supercapacitor. Synthesized aerogels were carbonized and then activated using carbon dioxide (CO₂) gas. The specific surface area and micropore size distribution were investigated by N₂/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and non-linear density functional theory method. The structural and morphological properties were investigated by X-ray diffraction (XRD) and scanning electron microscope (SEM), respectively. The hydrogen uptakes were analyzed at 77 K and 1 bar. Electrochemical behaviors were investigated by cyclic voltammetry (CV) in a three-electrode system. From the results, it was found that surface characteristics and porosities played an important role in the capacitance of electrode and hydrogen uptakes.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Preparation and Characterization of Silica-Templated Porous Carbons Derived from Polythiophene for Hydrogen Storage

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, porous carbons have been prepared by silica-templating method using MCM-41 as silica source and polythiophene as sulfur(S)-containing carbon precursor. The morphological properties were performed using a field emission transmission electron microscopy (FE-TEM). The textural properties were performed by N₂/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. The hydrogen uptake experiment was measured by a volumetric measurement at 77 K and 1 bar. The synthesized porous carbons obtained large specific surface area and hydrogen storage capacity (1.38 wt%). The results indicated that polythiophene-derived porous carbons could be attractive hydrogen storage materials.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Simulation of thermal equilibrium mixture compositions in hydrogen, benzene, and pristine or P-doped MoS₂ clusters related with clusters' catalytic capabilities in hydrocracking of vacuum residue from crude oil distillation

Hyo Weon Jang

Department of Chemistry, Sunchon National University, Korea

In this work, small model clusters of MoS₂ and its P-doped one are allowed to form various hydrogen- and/or benzene-bound clusters in the presence of H₂ and benzene, mimicking the initial stage of vacuum residue hydrocracking industrial process. DFT simulation results indicate that both clusters bind three benzenes and that the pristine cluster binds three additional H₂ molecules while the P-doped one binds four additional H₂ molecules at temperature of 700K and H₂ pressure of 120atm. This is in line with the experimental finding that the P-doped cluster produces less coke than the pristine cluster when they are used as hydrocracking catalysts, because we might think that the more H₂ bound to the cluster the more cracking feasible, eventually less coke in the final product. Their catalytic differences may be related with our finding that the sequential gaining of enthalpy as H₂ binds one by one remains almost constant for pristine cluster, while it decreases for the case of P-doped one.

Poster Presentation : **IND.P-18**

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

A Study on Polymerization Process of Polyethylene Wax with Low Molecular Weight Distribution and Small Molecular Weight by Polymerization Condition and Metallocene Catalyst Control

Intae Kim^{*}, Ji Woong Han

Department of Chemistry, Kwangwoon University, Korea

In this study, a polyethylene wax having a low molecular weight and a narrow molecular weight distribution was prepared by controlling various polymerization conditions such as temperature, hydrogen ratio, ethylene gas amount and polymerization pressure using various metallocene catalysts. Polyethylene waxes with very uniform physical properties polymerized through new methods can be effectively applied as coatings and Expanded Polystyrene (EPS) cell sizers. The physical properties of the wax were confirmed by measuring Number average molecular weight(Mn), Weight-average molecular weight(MW) and Poly Dispersity Index(PDI) data of the polymerized polyethylene wax through Gel Permeation Chromatography(GPC).

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Effect of pore and surface properties of titania materials on adsorption of heavy metals from water

Yeong-rae Son, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Water contamination by effluent from industrial plants has been seriously considered as a global problem. Among the various sources of water pollution, the heavy metal ions dissolved in water are harmful and toxic to living beings. Therefore, to remove the heavy metals from water, various methods have been applied. Among the methods, the adsorption has been highlighted owing to ease of high efficiency and low cost. In this study, the removal behaviors of various heavy metals in water, such as chromium, selenium, manganese, and zinc, were investigated using commercial titania materials with different porosity and surface properties. No specific differences in crystal structure and morphology of the titania materials investigated by X-ray diffraction and scanning electron microscopy were confirmed. The porosity of the titania materials, such as specific surface area, pore volume, and pore size distribution, was elucidated from N₂ adsorption-desorption isotherms. Zeta potential of the materials was measured to verify surface charge of the titania materials with different properties. The titania materials what we investigated have different mesopore volumes, pore sizes, and surface charges. It was found that the porosity and surface characteristics were a key point for the removal of heavy metals from water.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Designing three-dimensional reduced graphene oxide/CNT foams from aqueous medium and their supercapacitive behaviors

Yeong-rae Son, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Intercalation of spacers and modification of the nano/microstructure have been studied extensively to solve the restacking problems associated with graphene. However, the existing methods of structure modification to generate 3-dimensional (3D) framework are complex and inefficient. In this study, 3D graphene oxide/carbon nanotube (GO/CNT) foams were prepared by integrating GO sheets and CNTs from water-ethanol system via freezing and lyophilization without using any other materials. The GO sheets acted as a dispersing agent for carbon nanotubes in water and ethanol inhibited ice crystal growth as the temperature of the aqueous solution decreased, leading to an eco-friendly preparation of 3D graphene-based foam. The prepared GO/CNT foam exhibited special characteristics, such as a sponge-like morphology and unique textural properties, owing to the insertion of CNTs between GO layers. The GO/CNT foam could be reduced by thermal treatment without deformation, resulting in electrically conductive graphene-based foam with 3D networks. Furthermore, a supercapacitor composed of the reduced foam as electrodes and GO membrane as separator with electrolyte permeability and insulating properties was fabricated. The resultant supercapacitor showed distinctive electrochemical behaviors including high rate capability and cycle behavior because the unique structure of the foam led to rapid electrolyte ion diffusion.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Preparation of carbon nanotube-reinforced carboxymethyl cellulose nanocomposite films from aqueous medium and their mechanical behaviors

Yeong-rae Son, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

As environmental pollution caused by non-biodegradable synthetic polymers increases, biodegradable polymers have attracted attention as alternatives to overcome the limitations of synthetic polymers obtained from petrochemicals. However, these biopolymer-based films show inferior mechanical properties. Therefore, inorganic or hydrophobic materials, such as clays and carbon materials, have been introduced into biopolymer-based films. In the present work, carbon nanotube-reinforced carboxymethyl cellulose (CMC/CNT) nanocomposites were prepared by a solution casting method. The CNTs can be homogeneously dispersed in water with the aid of CMC polymer and was used as reinforcement. The crystal structure and morphologies of pure CMC, CNTs, and CMC/CNT nanocomposites were investigated by X-ray diffraction, transmission electron microscopy, and scanning electron microscope, respectively. The mechanical behaviors, tensile strength and Young's modulus, of the CMC/CNT nanocomposite films were estimated by universal testing machine after cutting films to specimens using ASTM D638-05 blade. As a result, the tensile strength and Young's modulus of CMC/CNT nanocomposites were enhanced by addition of the CNT owing to π - π interfacial interaction between CNT and CMC polymer chain.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Understanding the photophysical change of geometric isomers of heteroleptic Ir(III) complexes

So-Yoen Kim, Dae won Cho^{*}, Sang Ook Kang, Ho-Jin Son^{*}

Department of Advanced Materials Chemistry, Korea University, Korea

We have synthesized heteroleptic Ir(III) complexes showing red phosphorescence, which can be separated as two geometrical isomers. Each isomer showed different absorption and emission spectral behaviours. The phosphorescence of the *cis* isomer is observed at shorter wavelengths than the *trans* one. The LUMOs of both isomers are at the same energy level, but the HOMO of the *cis* isomer is shifted to a significantly lower energy than that of the *trans* isomer. The red emissions originate from the triplet metal-to-ligand charge transfer (MLCT) state, which is assigned by femtosecond time-resolved transient absorption spectroscopic analysis. The MLCT emission spectra of both isomers show highly structured bands with a vibronic spacing of ca. 1470 cm⁻¹. Observation of vibrational fine structure in the emission spectra is attributed to the limited excited state structural change imposed by the rigidity of metal coordination.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Bulky-substituent effect on excimer formation of square planar Pt(II) complexes

So-Yoen Kim, Jae-Hyun Park, Sang Ook Kang, Dae won Cho*, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In order to understand the steric influence on excimer formation in square planar metal complexes, three different Pt(II) complexes were prepared by modifying the substituents in the main ligand: Pt(II)(dfppy)(acac) (**Pt-1**, where dfppy is difluorophenylpyridine, acac is acetylacetonate); the bulky triphenyl silyl (Ph₃Si-) group was substituted at the pyridine moiety (**Pt-2**) and at the phenyl moiety (**Pt-3**) of the main ligand of **Pt-1**. The Pt-complexes showed sky-blue emission at ~460 nm. In addition, **Pt-1** and **Pt-3** showed excimer emission at ~600 nm in the concentrated solution and the solid sample. The emission lifetimes and intensities for monomeric **Pt-1** and **Pt-3** showed strong concentration dependence. Indeed, the lifetime of the monomer was reduced in highly concentrated solutions due to excimer formation. The intrinsic emission lifetimes were determined as 364 ns (**Pt-1**) and 300 ns (**Pt-3**) by Stern–Volmer analysis, considering the self-quenched lifetime of monomer emission. **Pt-2** did not show any excimer emission in the concentrated solution or solid sample. The crystal structures of **Pt-1** and **Pt-3** were analysed by X-ray crystallographic measurements. The results revealed that the LUMO moiety closely overlapped with that of another Pt-complex. In this study, based on the influence of steric hindrance of the bulky Ph₃Si group, we concluded that the LUMO–LUMO interaction between the pyridine moieties of the main ligand is the main factor responsible for excimer formation.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and characterization of heteroleptic cyclometalated Ir(III) complexes substituted with 2-(2-sulfonylfluorophenyl)pyridine (ppySO₂F) ligand for blue phosphorescent organic-light-emitting diodes

Jin-Hyoung Kim, So-Yoen Kim, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In order to understand the intrinsic nature of nonradiative processes in heteroleptic cyclometalated Ir(III) complexes, highly phosphorescent Ir³⁺ complexes containing 2-(2-sulfonylfluorophenyl)pyridine (ppySO₂F) as the cyclometalated ligand were newly synthesized. Three ancillary ligands, acetylacetonate (acac), picolinate (pic), and *tetrakis*-pyrazolyl borate (bor), were employed for the preparation of the Ir(III) complexes [Ir(ppySO₂F)₂(acac)] (**Ir-acac**), [Ir(ppySO₂F)₂(pic)] (**Ir-pic**), and [Ir(ppySO₂F)₂(bor)] (**Ir-bor**). The molecular structures were characterized by X-ray crystallography. Blue phosphorescence maxima were observed at 458, 466, and 478 nm for Ir-bor, Ir-pic, and Ir-acac, respectively, at 77 K, and the corresponding emission quantum yields were determined to be 0.79, 0.80, and 0.98 in anaerobic CH₂Cl₂ at 300 K. Additionally, the phosphorescence decay times were measured to be 1.27, 2.11, and 3.58 μs for **Ir-acac**, **Ir-pic**, and **Ir-bor**, respectively. No temperature dependence was observed for the emission lifetimes in 298-338 K. These results indicate that there is no activation barrier to crossing to a nonradiative state like metal-centered (MC, *d-d*) state. The radiative rate constants (*k_r*) are within a narrow range of 3.0–5.5 × 10⁵ s⁻¹. However, the nonradiative rate constants (*k_{nr}*) are within a wide range of 14.2–0.52 × 10⁴ s⁻¹. The *k_{nr}* values showed linear correlation with the energy gap. We carried out *ab initio* calculations to evaluate the energy states and their corresponding orbitals. The nonemissive MC states lie at higher energies than the emissive MLCT state, hence the MC states can be excluded from the nonradiative pathway.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

A study on electromagnetic interference shielding effectiveness of nickel-plated carbon fiber papers

Yoon-Ji Yim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

To develop high-quality electromagnetic interference shielding efficiency (EMI SE) materials, nickel plated-carbon fiber papers (Ni-CPs) were prepared using an electroless nickel-plating method and a wet-laid process to obtain Ni-CPs with enhanced EMI SE. The morphologies and structural properties of Ni-CPs were determined using scanning electron microscopy (SEM) and X-ray diffraction (XRD). It was found that the intensity of the metallic Ni peak increased with increasing Ni-plating time. In the frequency range of the electromagnetic waves from electrical appliances (0.5–1.0 GHz), the 5Ni-CPs exhibited high EMI SE. The EMI SE of the CPs was measured according to ASTM D4935-99 and increased in proportion to the current density because of the role of Ni particles. This result implies that the presence of Ni on the carbon fibers can lead to good EMI SE, owing to the EMI adsorption behaviors of the metal particles.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Electromagnetic Interference Shielding Effectiveness of Silver-plated MWCNTs/Epoxy Composites

Yoon-Ji Yim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Multi-walled carbon nanotubes (MWCNTs) were silver (Ag)-plated chemically to enhance the electromagnetic interference shielding effectiveness of Ag-MWCNTs/Epoxy composites. The morphological properties of the Ag-MWCNTs were characterized by scanning electron microscopy (SEM). The micro-structural and surface characteristics of the Ag-MWCNTs were examined by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS), respectively. The EMI SE of the Ag-MWCNTs/Epoxy composites was tested by EMI shielding analyzer. From these results, the higher Ag content on the MWCNTs of the composites showed a better EMI SE. The EMI-SE of Ag-MWCNTs/Epoxy composites were measured to be 10 dB from 1 GHz band, which was increased compared to that of the as-received MWCNTs (7 dB). This indicates that the presence of Ag on the MWCNTs can lead to a good EMI-SE due to the EMI adsorption behavior of the metal particles.

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

Industrial Chemistry

Grand Ballroom, FRI 11:00~12:30

Freeze Protected Sanitary Liquid for Winter-season

Heeseok Woo, Gyoyoon Chae, Jae Ku Jung, Won-Seok Chae*

Division of Life Science and Chemistry, Daejin University, Korea

A sanitary liquid was prepared to prevent freezing in winter. The solution is a hygiene solution containing alcohols as a main component and a surfactant added thereto. 25% and 15% of ethanol and isopropyl alcohol were mixed, respectively, and 1% of benzalkonium chloride was added as a surfactant. The solution did not freeze for 48 hours at a temperature of minus 30 degrees. In addition, the solutions diluted to 75% and 50% did not freeze at -20 and -10° C, respectively. The concentration at which ethanol does not freeze at about -30 ° C is about 50%, and isopropyl alcohol is about 70%. However, when the two solvents were mixed with water, they did not freeze even at the lower concentration due to the synergistic effect of the colligative properties of a solution. The solution diluted to 25% was showed the 99.9% sterilizing power against *Escherichia coli*, *Pseudomonas aeruginosa*, *Pneumococcus*, *Salmonella*.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Reactions of dialkyl Pd(II) and Pt(II) complexes with organic tetrazole-thiones

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¹*Chemistry, Gangneung-Wonju National University, Korea*

²*Department of Chemistry, Sungkyunkwan University, Korea*

Various tetrazole-thiolato Pd(II) or Pt(II) complexes were obtained from the reactions of trans-PdEt₂(PR₃)₂ or cis-PtEt₂(PR₃)₂ with organic tetrazole-thiones {S=[C{HN₄(R)}]}. The isolated complexes were determined by IR and NMR spectroscopy and X-crystallographic analyses. Treatments of alkyl Pd(II) or Pt(II) tetrazole-thiolato complexes with another {S=[C{HN₄(R)}]} afforded corresponding new bis(tetrazole-thiolato) Pd or Pt(II) complexes. Experimental detail will be discussed.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Reactivity of group 10 zero-valent complexes toward organic isocyanates

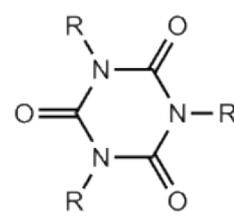
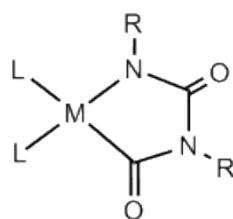
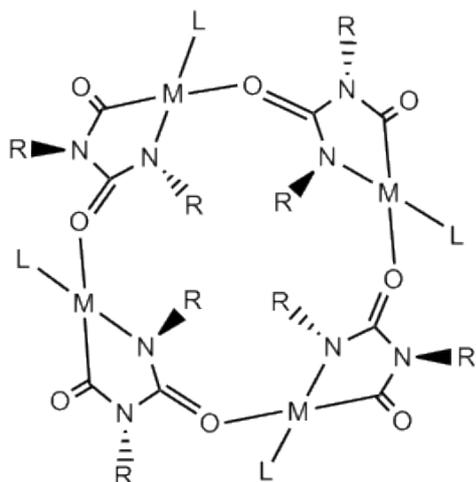
Yong-Joo Kim^{*}, Young-sung Han¹, Kang Yeoun Jung¹, Soon W. Lee²

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Group 10 (Ni, Pd, and Pt) zero-valent complexes reacted with two equivalent or excess amounts of organic isocyanates. Isolated compounds were characterized by IR, NMR and GC-MS. Chemical reactions or catalytic properties of the isolated complexes with excess R-NCO were performed. Experimental details will be discussed.



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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

**Polyhedral oligomeric silsesquioxane-conjugated
bis(diphenylphosphino)amine ligand for chromium(III) catalyzed
ethylene trimerization and tetramerization**

Hoseong Lee, Soon Hyeok Hong*

Division of Chemistry, Seoul National University, Korea

Polyhedral oligomeric silsesquioxanes (POSSs) were attached to conventional bis(diphenylphosphino)amine(PNP) ligand as solubility-enhancing materials for catalytic ethylene trimerization and tetramerization. Differently functionalized arylphosphine ligands of the type (Ph)₂PN(POSS)P(Ph)(ArR) (R=functional groups) were systematically developed, and their corresponding chromium(III) complexes were formed. The developed precatalysts exhibited excellent tolerance in solvents, including even low-carbon-number hydrocarbons such as n-pentane, n-hexane, or cyclohexane. In particular, the ortho-fluorophenyl-substituted complex showed higher stability even at higher temperatures above 120 °C. The ortho-OCF₃-phenyl-substituted complex showed outstanding catalytic activity, which reached 2287 kg/g Cr/h at 30 bar.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of Hypercrosslinked Porous Organic Polymers having Densely Acidic and hydrophobic Surface via Post-synthetic modifications

**Dong Won Kang, Minjung Kang, Sunhwi Eom, Jong Hyeak Choe, Jeoung Ryul Park¹,
Hyojin Kim², Daewon Kim³, Chang Seop Hong***

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We prepared a hypercrosslinked porous organic polymer, **1T**, and sequentially modified it to **1TC** and **1TCS**. Carboxylic groups of **1TC** were oxidized from methyl groups of **1T** and sulfonic acid groups of **1TCS** were introduced from **1TC** via direct substitution using chlorosulfonic acid. The compounds were characterized by different techniques including infrared spectroscopy, thermogravimetric analysis, X-ray photoelectron spectroscopy, ¹³C Solid state nuclear magnetic resonance, gas sorption and impedance spectroscopy. Especially, **1TCS** showed the highest ammonia capture capability per surface area. To enhance selective NH₃ adsorption over water vapor, we coated the surface of **1TCS** with hydroxyl-terminated poly(dimethylsiloxane) (PDMS). As a result, **1TCS@PDMS10** showed enhanced NH₃ adsorption capacity at the low pressure and hydrophobicity. Detailed contents will be given in the poster presentation.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Surface modification of $Mg_2(m\text{-dobdc})$ with PDMS and its applications

Sunhwi Eom, Dong Won Kang, Minjung Kang, Jong Hyeak Choe, Hyojin Kim¹, Jeoung Ryul Park², Daewon Kim³, Chang Seop Hong^{*}

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We prepared $Mg_2(m\text{-dobdc})$ ($m\text{-dobdc}^{4-} = 4,6\text{-dioxido-1,3-dibenzenedicarboxylate}$), featuring exposed metal cation sites with a higher apparent charge density. To improve moisture resistance and hydrophobicity, hydrophobic polymer PDMS (polydimethylsiloxane) was coated to MOF. The properties of compounds were analyzed by various techniques including infrared spectroscopy, thermogravimetric analysis, powder X-ray diffraction, gas sorption and water contact angle. Detailed synthetic scheme and several properties will be given in the presentation.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication and Characterization of a Metal-Organic Framework-Composite with Filter Paper

Hyojin Kim, Dong Won Kang¹, Minjung Kang¹, Sunhwi Eom¹, Jong Hyeak Choe¹, Jeoung Ryul Park², Daewon Kim³, Chang Seop Hong^{1,*}

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The development of MOF-composite (MOF; Metal-Organic Framework) with a filter paper is a valuable strategy for the effective applications of metal-organic framework powder. To begin with, we prepared a carboxymethylated filter paper to enhance the number of nucleation sites for the MOF growth on the paper and Mg₂(dobpdc) (H₄dobpdc; 4,4'-Dihydroxy-[1,1'-biphenyl]-3,3'-dicarboxylic acid) nanoparticles were grown on the carboxymethylated filter paper. Subsequently, we coated the surface of Mg₂(dobpdc)-paper with hydroxyl-terminated poly(dimethylsiloxane) (PDMS) to maintain the flexibility of filter paper. Mg₂(dobpdc)-paper was characterized by infrared spectroscopy, thermogravimetric analysis, powder X-ray diffraction, and scanning electron microscope. Detailed synthetic scheme and characterization will be presented in the poster.

Poster Presentation : **INOR.P-34**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

**Zintl Phase Thermoelectric Material with the *n*-type dopant:
 $\text{Ca}_{3.40(3)}\text{Yb}_{1.48}\text{Pr}_{0.12}\text{Al}_2\text{Sb}_6$**

Seungeun Shin, Tae-Soo You*

Department of Chemistry, Chungbuk National University, Korea

Thermoelectric (TE) materials and the devices based on these materials have been considered as one of the smartest approaches to reduce global energy consumption by recovering the wasted heat from various heat sources and converting it into electricity. Recently, the $A_5M_2Pn_6$ ($A = \text{Ca}, \text{Sr}, \text{Eu}, \text{Yb}, M = \text{Al}, \text{Ga}, \text{In}$) series has been extensively investigated as Zintl phase TE materials, and two major structure types have been identified: the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type having metallic behavior and the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type showing the semiconducting behavior. To investigate the effect of cationic substitution and *n*-type doping for TE properties of the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type compounds, a quinary Zintl phase $\text{Ca}_{3.40(3)}\text{Yb}_{1.48}\text{Pr}_{0.12}\text{Al}_2\text{Sb}_6$ was successfully synthesized by arc-melting, and its crystal structure was characterized by both powder and single-crystal X-ray diffractions. It is already known that in the $\text{Ca}_{5-x}\text{Yb}_x\text{Al}_2\text{Sb}_6$ ($1.0 \leq x \leq 5.0$) system, the Ca-rich compounds adopt the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type structure through the post heat treatment. Nevertheless, the title compound adopted the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type with the orthorhombic space group *Pbam* ($Z = 2$, Pearson Code *oP26*) even after the post heat treatment despite of its Ca-rich composition. According to the SXRD result, the symmetrically independent cationic sites contain a $\text{Ca}^{2+}/\text{Yb}^{2+}$ mixed-occupation with various mixed ratios. In particular, one cationic site additionally contains the *n*-type dopant Pr^{3+} . Based on the deviation from the previously reported structural transformation trend, to understand the difference induced by *n*-type doping, a series of theoretical calculations using three different hypothetical structural models by tight-binding linear muffin-tin orbital method were performed and the results are thoroughly analyzed.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Quantum dots-based fluorescence sensor for sensitive detection of hydrogen peroxide

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¹Advanced Analysis Center, Korea Institute of Science and Technology, Korea

Quantum dots are being developed for a various kind of applications. We use quantum dots for hydrogen peroxide sensor because of their high brightness and high luminescence. Transmission electron microscopy (TEM) characterizations indicate that the size of quantum dots are about 5–10 nm, respectively. The quantum dots showed strong orange luminescence under irradiation with ultra-violet light. For this Quantum dot, the excitation peak was 222 nm and the emission peak was 600 nm. As the concentration of hydrogen peroxide increased, the fluorescence intensity of the emission peak decreased. The optimal conditions such as pH, temperature in solution stimulated to a more rapid quenching phenomenon in the optimized quantum dot system. The fluorescence intensity ratios of the optimized quantum dot solution exhibited a linear correlation with the hydrogen peroxide with concentrations ($y=-0.50762x+443.7775$, $r^2=0.96068$) This sensor has high property and can selectively detect hydrogen peroxide.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Minor Structural Variations of Small Molecules Tune Regulatory Activities toward Pathological Factors in Alzheimer's Disease

Mingeun Kim, Mi Hee Lim^{1,*}

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Chemical tools have been valuable for establishing a better understanding of the relationships between metal ion dyshomeostasis, the abnormal aggregation and accumulation of amyloid- β ($A\beta$), and oxidative stress in Alzheimer's disease (AD). Still, very little information is available to correlate the structures of chemical tools with specific reactivities used to uncover such relationships. Recently, slight structural variations to the framework of a chemical tool were found to drastically determine the tool's reactivities toward multiple pathological facets to various extents. In this presentation, we will present our rational design and characterization of a structural series to illustrate the extent to which the reactivities of small molecules vary toward different targets as a result of minor structural modifications. These compounds were rationally and systematically modified based on consideration of properties, including ionization potentials and metal binding, to afford their desired reactivities with pathological factors in AD. Together, our studies demonstrate the rational structure-directed design that can be used to develop chemical tools capable of regulating individual or interrelated pathological features in AD.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

A new breathing three-dimensional Zn-MOF with Lewis basic nitrogen-rich channels: selective carbon dioxide sorption

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Openly accessible Lewis basic sites orderly located inside the well-defined channels of metal–organic frameworks (MOFs) are potentially ideal active sites for selective gas sorption and catalysis. A new C₂h-symmetric dicarboxylate-based bridging ligand, 3,3'-(pyrazine-2,5-diyl)dibenzoic acid (3,3'-PDBA) was prepared by a Suzuki coupling reaction, and two new Zn-MOFs containing the C₂h-symmetric 3,3'-PDBA bridging ligand and two different bis(pyridyl)-based pillars (1,2-bis(4-pyridyl)ethane (bpa) or 1,2-bis(4-pyridyl)ethylene (bpe)) were prepared through a thermal reaction in DMF. Two Zn-MOFs of the general formula of three-dimensional (3D) [Zn₂(μ₄-3,3'-PDBA)₂(μ₂-bpa)]₃·(DMF)₅(H₂O)₁₃ (**1**) or 3D-like 2D [Zn₂(μ₄-3,3'-PDBA)₂(μ₂-bpe)]·(H₂O) (**2**) with primitive cubic pcu net and 2D sql net, respectively. Both Zn-MOFs **1** and **2** contain uncoordinated Lewis basic pyrazinyl nitrogen atoms in the frameworks. Zn-MOF **1** with openly accessible Lewis basic sites exhibited selective sorption of CO₂ over N₂, H₂, and CH₄ at low temperature. The adsorption and desorption isotherms for CO₂ sorption at 196 K showed phenomenal hysteretic behaviour indicative of a breathing process through an adsorbate-discriminatory gate-opening process toward CO₂ at a low gas pressure.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of hydrophobic flexible free-standing titanium carbide (Ti₃C₂T_x) MXene coated carbon fabric for EMI shielding in S band region

Raagulan Kanthasamy, Gyu Youn Chea^{1,*}, Bo Mi Kim¹, Seon Guk¹

Chemistry, Wonkwang University, Korea

¹*Department of Chemistry, Wonkwang University, Korea*

Electromagnetic interference (EMI) is a worldwide issue due to the modern electronic systems. MXene, is graphene like two-dimensional material is an attractive candidate for EMI shielding material along with non-woven carbon fabric is an excellent choice as carbon base material. The MXene coated fabric was fabricated by facile dip coating process and structural features, EMI shielding effectiveness, electric conductivity and wettability were investigated. The coating process generated hydrophobic surface with contact angle of 123°, wetting energy of -39.86 mN/m, 33mN/m work of adhesion and spreading Coefficient of -113mN/m. The composites exhibit excellent thermal stability until 250°C with 5 % weight loss between 250 to 350°C temperature range. The 15-times coated (D15) exhibited higher EMI shielding effectiveness about 43 dB at 2.3 GHz with absolute EMI shielding of 7734.5 dBcm²g⁻¹ and 247.5 dBcm³g⁻¹ shielding effectiveness. The changes of EMI shielding effectiveness of composite was 1 dB/cycle. According to the above result, composite display better outlook application areas like aviation, portable electronics, radars, aerospace and military.

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

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of MWCNT Coated flexible free-standing Carbon Fabric composite with Higher Absolute EMI SE

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MWCNT coated carbon fabrics composite were fabricated by using facile dip coating process. The thickness and fissures of the fabrics were altered by using oxidized MWCNT/SDS dispersed solution. The coating process significantly affect the tensile strength, electrical conductivity, EMI shielding of the composites. The composite exhibit excellent thermal restrains up to 284°C with 0.63 W-1K-1 maximum thermal conductivity. The composite displayed 16.42 S cm⁻¹ higher electrical conductivity with 3.3 Ω/sq low sheet resistance. 68 dB of highest EMI shielding shown double layer fabric at 2.7 GHZ whereas singly coated fabric exhibited 37 dB maximum EMI shielding at 2 GHz with 486.54 dBcm³g⁻¹ specific SE and 35000 dBcm²g⁻¹ absolute SE. According to the above-mentioned results leads the composite for the potential shielding applications such as aeronautic, military, automobile and portable electronic devices.

Poster Presentation : **INOR.P-40**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

EMI shielding of titanium carbide (Ti₃C₂T_x)-carbon nanotube-SDS coated light weight, flexible and free-standing composite fabric in S band region.

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Chemistry, Wonkwang University, Korea

¹*Department of Chemistry, Wonkwang University, Korea*

²*Wonkwang University, Korea*

The sequence of thin MXene-CNTO-SDS coated wet laid non-woven carbon fabric was manufactured with low density and low porosity. The fabricated composite was characterized using X-ray diffraction (XRD), scanning electron microscope (SEM), Raman spectroscopy, energy dispersive X-ray (EDX) and X-ray photoelectron spectroscopy (XPS). The fabricated composite showed excellent electric conductivity of 12.8 S/cm with lower sheet resistance 2.75 Ω/sq. The composite exhibited excellent thermal stability and constrained the degradation until 200°C with 8% of weight loss between 200 to 500° temperature range. Twenty-five times coated carbon fabric (MXCNTC25) displayed highest EMI shielding approximately 40 dB at 2.3 GHz with specific EMI shielding (SSE) of 214 dBcm³g⁻¹ and absolute EMI shielding (SSE/t) 7523.78 dBcm²g⁻¹. According to aforementioned above result, the fabricated composite displays excellent properties towards the application areas like mobile phones, aeronautics, radars and military applications.

Poster Presentation : **INOR.P-41**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

EMI shielding of Titanium Carbide (Ti₃C₂T_x)- graphene-polymer thin film and Hydrophobic, flexible, freestanding Graphene-PVDF coated carbon fabric composite in S band region.

Raagulan Kanthasamy, Braveenth Ramanaskanda¹, Gyu Youn Chea^{1,*}, Bo Mi Kim¹, Leero Lee²

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MXene is a layered two-dimensional material like graphene is an attractive candidate for electromagnetic interference shielding. MXene and graphene based thin, flexible and low-density polyvinylidene fluoride(PVDF)- Polyacrylic acid (PAA) composite were prepared by coast effective spray coating and solvent casting method. The fabricated composite characterized using X-ray diffraction (XRD), X-ray photoelectron spectroscopy(XPS), Raman measurement, energy dispersive X-ray (EDX) and scanning electron microscope (SEM). The fabricated composites displayed hydrophobic nature with uppermost 126° contact angle, -116 mN/m spreading Coefficient, 30 mN/m lowest work of adhesion and -43 mN/m wetting energy. The composites displayed excellent conductivity of 13.68 S/cm with sheet resistance of 3.1 Ω/sq. All the composite truncated intense weight lost up to 400°C and exhibited outstanding thermal stability. The MXene-graphene foam showed 41 dB of excellent EMI shielding at 2.97 GHz frequency range with 36 dB average EMI shielding and 1324.29 dBcm²g⁻¹ absolute shielding effectiveness. Mono layer graphene coated carbon fabric exhibited exceptional absolute shielding effectiveness of 35370 dBcm²g⁻¹ with shielding effectiveness of 453 dBcm²g⁻¹ and 33 dB of maximum EMI shielding at 2.17 GHz. Hence, above results standpoint the applications such as handy electronics, mobile phones, aeronautics, air travels, radars, and military applications.

Poster Presentation : **INOR.P-42**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cadmium coordinated trimeric concanavalin A from *Canavalia ensiformis*

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Rapid methods for the detection and clinical treatment of human norovirus (HuNoV) are needed to control foodborne disease outbreaks, but reliable techniques that are fast and sensitive enough to detect small amounts of HuNoV in food and aquatic environments are not yet available. We explore the interaction between HuNoV and concanavalin A (Con A), which could facilitate the development of a sensitive detection tool for HuNoV. Biophysical studies including hydrogen/deuterium exchange (HDX) mass spectrometry and surface plasmon resonance (SPR) revealed that when the metal coordinated region of Con A, which spans Asp16 to His24, is converted to nine alanine residues (mCon AMCR), the affinity for HuNoV (GII.4) diminishes, demonstrating that this Ca²⁺ and Mn²⁺ coordinated region is responsible for the observed virus-protein interaction. The mutated carbohydrate binding region of Con A (mCon ACBR) does not affect binding affinity, indicating that MCR is a major region of interaction. The results further contribute for the development of a HuNoV concentration tool, Con A-immobilized polyacrylate beads (Con A-PAB), for rapid detection of genotypes of genogroup I and II (GI and GII). This method offers many advantages over currently available methods, including a short concentration time. Norovirus can be detected in just 15 minutes with 90% recovery through Con A-PAB application. In addition, this method can be used over a wide range of pH values (pH 3.0– 10.0). Overall, this rapid and sensitive detection of human norovirus will aid in the prevention of virus transmission pathways and the method developed here may have broad applicability for other foodborne viral infections.

Poster Presentation : **INOR.P-43**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Catalytic roles of zinc finger proteins with structural integration

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Zinc finger (ZF) proteins use zinc as a structural co-factor and are often involved in nucleic acid recognition and binding. Although zinc is typically thought to be the physiologically relevant transition-metal ion for ZF protein function, there is evidence that other metal ions, including iron, may replace zinc under certain conditions. Studies focused on the roles of metal coordination and DNA binding for two specific ZF proteins: ST18 (suppression of tumorigenicity 18) and ZIF268 (zinc interacting factor 268) will be presented. ST18 is a non-classical ZF that belongs to the NZF/MyT family of ZFs. It contains six ZF domains, each of which has a Cys2His2Cys motif. The biological function of ST18 is not well understood; however, there is some recent evidence that ST18 regulates inflammation and apoptosis by regulating gene expression of tumor necrosis factor- α (TNF- α). We have been studying constructs of ST18 that contain the Cys2His2Cys domains, and have obtained evidence for zinc binding. These studies along with DNA binding studies with the TNF- α promoter will be presented.

Poster Presentation : **INOR.P-44**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Experimental and Theoretical Investigations for the n-doping Effects in the $\text{Ca}_{11-x}\text{RE}_x\text{Sb}_{10-y}$ (RE = Gd-Tm; $0.32(3) \leq x \leq 0.43(2)$, $0.19(1) \leq y \leq 0.51(1)$) Series

JunSu Lee, Tae-Soo You*

Department of Chemistry, Chungbuk National University, Korea

We recently reported the n-type dopant included novel Zintl phase $\text{Ca}_{11-x}\text{RE}_x\text{Sb}_{10-y}$ (RE = La, Ce, Nd, Sm; $0.18(4) \leq x \leq 0.42(2)$, $0.14(1) \leq y \leq 0.41(1)$) system adopting the $\text{Ho}_{11}\text{Ge}_{10}$ -type structure for thermoelectric application. As an extension of the research, we present a successive work including other n-type dopants in the $\text{Ca}_{11-x}\text{RE}_x\text{Sb}_{10-y}$ (RE = Gd-Tm; $0.32(3) \leq x \leq 0.43(2)$, $0.19(1) \leq y \leq 0.51(1)$) system. Total six ternary Zintl compounds were successfully synthesized by arc-melting, and their crystal structures were characterized by both PXRD and SXR D analyses. In particular, two SXR D data of $\text{Ca}_{10.60(4)}\text{Ho}_{0.40}\text{Sb}_{9.69(1)}$ and $\text{Ca}_{10.57(2)}\text{Tm}_{0.43}\text{Sb}_{9.63(1)}$ were collected using synchrotron X-ray diffraction to obtain the further accurate structural information. All six compounds showed an isotypic crystal structures, which adopted the tetragonal $\text{Ho}_{11}\text{Ge}_{10}$ -type structure (space group $I4/mmm$, $Z = 4$, Pearson code $tI84$) and contained nine crystallographically independent asymmetric atomic sites in a unit cell. To understand the overall electronic structure as well as chemical bonding, tight-binding linear muffin-tin orbital (TB-LMTO) calculations were performed using a hypothetical structural model of $\text{Ca}_{10.5}\text{RE}_{0.5}\text{Sb}_{10}$ (RE = Dy, Ho), and density of states (DOS) and crystal orbital Hamilton population (COHP) curves were thoroughly interrogated. The temperature-dependent dc magnetization was also measured between 15 and 300 K under ZFC and FC conditions with a dc magnetic field of 10 kOe for three compounds including $\text{Ca}_{10.35(9)}\text{Dy}_{0.58}\text{Sb}_{9.53(3)}$, $\text{Ca}_{10.60(4)}\text{Ho}_{0.40}\text{Sb}_{9.69(1)}$ and $\text{Ca}_{10.68(3)}\text{Er}_{0.32}\text{Sb}_{9.50(1)}$.

Poster Presentation : **INOR.P-45**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

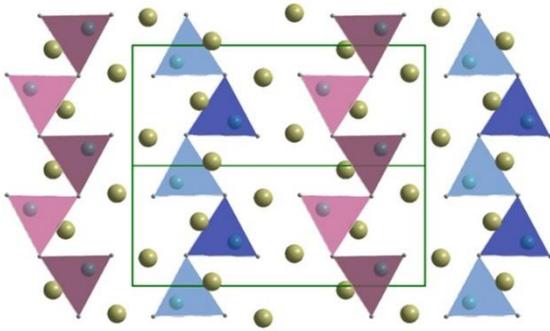
Zintl Phase with the Mixed Cations for the Thermoelectric Material Application: the Series of $\text{Ca}_{2-x}\text{Yb}_x\text{CdSb}_2$

Ki Won Kim, Tae-Soo You*

Department of Chemistry, Chungbuk National University, Korea

Recently, it was reported that the novel thermoelectric Zintl compound in the $\text{Yb}_{2-x}\text{Eu}_x\text{CdSb}_2$ system adopting the Yb_2CdSb_2 -type structure showed decent ZT values. However, the cationic mixing of Ca^{2+} and Yb^{2+} has not been reported yet. In addition, considering previously known two Zintl phases the Ca_2CdSb_2 and the Yb_2CdSb_2 compounds, the $\text{Ca}^{2+}/\text{Yb}^{2+}$ cation mixing can provide some interesting perspectives for the Zintl phase TE materials. Thus, a series of $\text{Ca}_{2-x}\text{Yb}_x\text{CdSb}_2$ compounds were synthesized by the Pb-flux reactions, and its crystal structure was characterized by both of the powder and single crystal X-ray diffractions. According to SXRD refinement, it was clear that the compounds having the relatively larger Ca content adopted the Ca_2CdSb_2 -type, while the compounds having the relatively larger Yb content adopted the Yb_2CdSb_2 -type structure. The Ca_2CdSb_2 -type structure adopts the orthorhombic space group $Pnma$, and the Yb_2CdSb_2 -type compounds crystallize in the $Cmc2_1$. In addition, both structures contain five independent atomic sites. Tight-binding linear muffin-tin orbital calculations were also performed to understand chemical bonding and the overall electronic structure. In this process, density of states and crystal orbital Hamilton population were thoroughly interrogated. As a result, the Ca_2CdSb_2 -type compound showed the semiconductor behavior with narrow band gap, while the Yb_2CdSb_2 -type displayed the poor metallic behavior with a pseudogap. Thermoelectric property measurements for these compounds are underway.

Pnma (Ca_2CdSb_2 -type)



Cmc2₁ (Yb_2CdSb_2 -type)

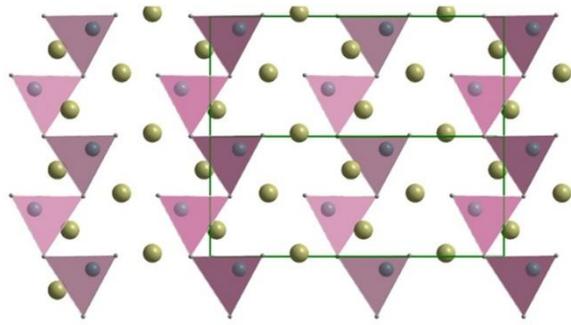


Figure 1. A schematic representation of the way the structure of Ca_2CdSb_2 -type and Yb_2CdSb_2 -type. Cd centered anionic network is presented by polyhedra

Poster Presentation : **INOR.P-46**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Exploration of catalytic selectivity in ethylene oligomerization: anchoring catalytic sites in a tailored metal-organic framework (MOF)

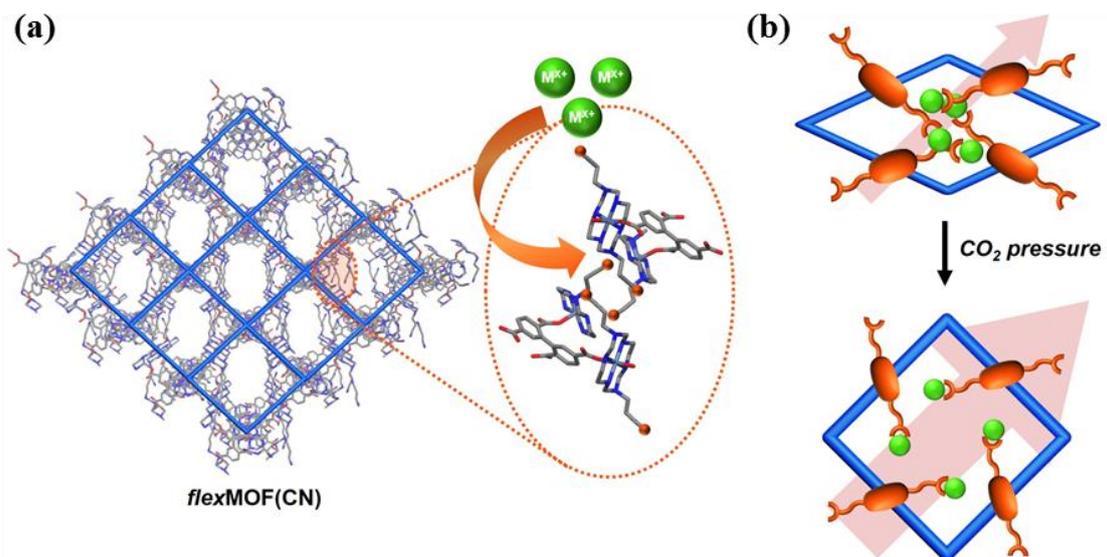
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Metal-organic frameworks (MOFs) have recently emerged as a promising platform for heterogeneous catalysts owing to their high surface area and tunability. Herein, we designed a MOF, *flex*MOF(CN) possessing free nitrile groups to anchor single-site catalyst. This *flex*MOF(CN) shows flexible behaviours such as gate-opening and breathing upon kinds and amounts of guest molecules, especially showing the structural transformation upon CO₂ pressure. With the active transition metals anchored to the MOF scaffold, we expected the synergistic effects of the flexible system on the catalytic reaction. Indeed, its flexibility resulted in interesting catalytic performance with selectivity upon reaction conditions in gas-phase ethylene oligomerization reaction. More importantly, in CO₂ atmosphere at the gate-opening pressure the catalytic conversion was significantly improved, and the selectivity was also changed. As a result, flexible MOFs can give an opportunity to control and enhance the catalytic performances by tuning specific reaction conditions.



Poster Presentation : **INOR.P-47**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

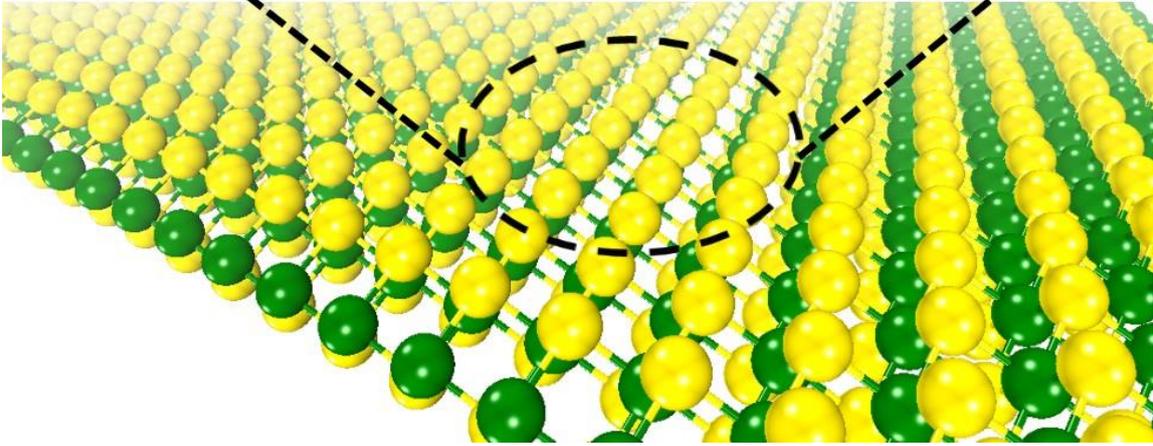
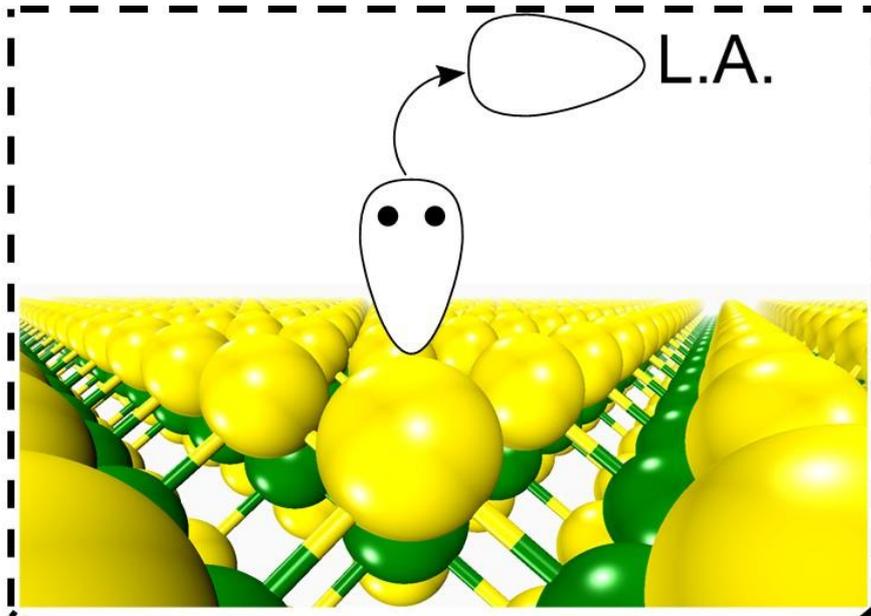
Selective Activation of the Basal Plane in Two Dimensional Transition Metal Chalcogenide Nanostructures

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¹Department of Chemistry, Yonsei University, Korea

Achieving a molecular level understanding of chemical reactions on the surface of solid-state nanomaterials is important but challenging. For example, two-dimensional (2D) layered transitionmetal chalcogenides (TMCs) can display unique reactivities due to their unusual anisotropic nature where the edges consisting of unsaturated metals and chalcogens may promote atomic rearrangement and catalysis, but the basal plane is believed to be rather inert and its surface chemistry is poorly explored. Herein, we show a molecular approach for selective activation of the basal plane on 2D layered TMCs using Lewis acids to initiate electrophilic addition selectively onto sulfide moieties, followed by transmetalation, which results in nanopores. This approach is generally operative not only in various compositions of TMCs, but also in crystal geometry such as 1T and 2H. Nanoporous NbS₂ materials obtained by this method was found to have an enhanced electrochemical energy storage capacity of 302 mF/cm², the highest reported to date for 2D nanostructure-based electrodes with longterm durability.



Poster Presentation : **INOR.P-48**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Their Photophysical Properties of Salen–Al/Triphenylamine (TPA) Assembly Dyads

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Triphenylamine (TPA)-based compounds have received much interest in versatile optoelectronic applications, such as organic photovoltaic cells (OPVs), organic light-emitting diodes (OLEDs), as the shape of small molecules and polymers. As a unique building block with electron-rich properties, the TPA molecule can be easily tuned with various functional groups, thus exhibiting interesting photophysical properties. We have recently reported the carbazole-containing salen–Al complexes, which showed the enhancement of the quantum efficiency by intramolecular energy transfer (IET) process. Based on the previous result, we newly designed and synthesized a novel class of salen–Al assembly dyads bearing TPA groups capable of acting as intramolecular energy host. The detailed synthesis, characterization, and optical properties of a series of salen–Al assembly dyads in conjunction with theoretical calculations will be described.

Poster Presentation : **INOR.P-49**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Preparation and application of mesoporous silica vesicles with large surface holes

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When the mesoporous silica nanoparticles are synthesized through self-assembly process, the cationic surfactant's role is paramountly important. Cetyltrimethylammonium bromide (CTAB) or cetylpyridinium bromide (CTPB) are well-known ammonium-based surfactants frequently used for mesoporous silicas. Meanwhile, there is a cationic surfactant that has a fluorocarbon chain like FC-4, and the chain is neither hydrophilic nor hydrophobic and is insoluble in water. In this study, mesoporous silica vesicles (MSVs) were successfully synthesized by using a binary mixed template system, CTPB and FC-4. In addition, the mesopore expansion and template-removal were simultaneously achieved by Ca ion-etching method using the as-prepared MSVs. The Ca ion-etching process effectively generated large surface holes through partial collapse of several mesopores. The Ca ion-etched MSV (Ca-MSV) showed better abilities encapsulating proteins compared to the calcined MSV with smaller mesopores. The Ca-MSV was especially good at adsorbing large size proteins such as hemoglobin, ovalbumin, and bovine serum albumin.

Poster Presentation : **INOR.P-50**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Optical and emission properties of cationic dyes captured in the mesoscale channels of metal-organic framework crystals

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

In this study, we exchanged $[\text{Et}_2\text{NH}_2]^+$ counter-cations in the anionic In-BTB metal-organic framework (MOF), $[\text{Et}_2\text{NH}_2]_3[\text{In}_3(\text{BTB})_4] \cdot 10\text{DEF} \cdot 14\text{H}_2\text{O}$, with a series of cationic dyes to prepare dye-encapsulated In-BTB MOFs (dye@In-BTBs). We chose six cationic dyes for the cation exchange: rhodamine 6 G (Rh6G), Nile blue A (NBA), Astrazon Orange G (AOG), crystal violet (CV), 3,3'-diethyloxycarbocyanine iodide (DEOCy), and 2-[4-dimethylamino]styryl)-1-methylpyridinium (DMMP). The cationic dyes have different geometries and physical dimensions. Six cationic dyes were easily exchanged with ammonium ions, and we successfully solved the crystal structures of six dye@In-BTBs. The confined spaces of In-BTB only allowed the dyes to contain structures somewhat different from free state. In addition, the distances between each captured dye were also different from the dyes in their solid states. Therefore, these differences led to unique photophysical properties of each dye compared to its free state. Detailed photophysical properties of the captured dye molecules will be presented.

Poster Presentation : **INOR.P-51**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Highly Selective and Durable Photochemical CO₂ Reduction by Molecular Mn(I) Catalyst Fixed on Particular Dye-Sensitized TiO₂ Platform

Pil Soo Kim, Sunghan Choi, So-Yoen Kim, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A new Mn(I)-based hybrid system (OrgD-[TiO₂]-MnP) for photocatalytic CO₂ reduction is designed to be a co-assembly of Mn(4,4'-Y2-bpy)(CO)₃Cl (MnP; Y = CH₂PO(OH)₂) and (E)-3-[5-(4-(diphenylamino)phenyl)-2,2'-bithiophen-2'-yl]-2-cyanoacrylic acid (OrgD) on TiO₂ semiconductor particles. The OrgD-[TiO₂]-MnP hybrid reveals persistent photocatalytic behavior, giving high turnover numbers and excellent product selectivity (HCOOH versus CO) which surpass the catalytic activities of related homogeneous and other heterogenized Mn photocatalytic systems reported so far. As a typical run, visible-light irradiation of the hybrid catalyst in the presence of 0.1 M electron donor (ED) and 0.001 M LiClO₄ produced persistently HCOOH with a >99% selectivity accompanied by a trace amount of CO; the turnover number (TON_{HCOOH}) reaches ~210 after 25 h irradiation. The product selectivity (HCOOH/CO) was found to be controlled by changing the loading amount of MnP on the TiO₂ surface. In-situ FTIR analysis of the hybrid during photocatalysis revealed that the Mn-H monomeric mechanism associated with HCOOH formation is dominated at low Mn concentration whereas CO is formed via an Mn-Mn dimer mechanism at high Mn concentration.

Poster Presentation : **INOR.P-52**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Efficient Photochemical Carbon Dioxide Reduction of a Molecular Re(I) Catalyst-Immobilized Porphyrinic Metal-Organic Frameworks (PCN-222) Inspired by Photosensitizer Array of Photosystem I

Sunghan Choi, So-Yoen Kim, Kyu Tai Park, Sang Ook Kang, Chul Hoon Kim*, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A porphyrinic metal-organic framework (PMOF) known as PCN-222 was surface-modified by the molecular Re(I) catalyst through anchoring to the outer layer with carboxylate to form a new type of MOF hybrid photocatalyst. The porphyrinic MOF-based hybrid (PMOF-Re) prepared with an archetypical CO₂ reduction catalyst, (L)ReI(CO)₃Cl (Re(I); L = 4,4'-dicarboxylic-2,2'-bipyridine), showed a high catalytic activity on CO₂ reduction with a long-term stability. A protective coating of TiO₂ grown with post-treatment atomic layer deposition of TiO₂ (TiO₂-AIM) further improved the catalytic durability of this hybrid as a result of ALD-engendered structural strengthening of MOF, with its role as an electron mediator transferring the photo-excited electrons of PMOF toward the Re(I) reaction center. In a typical run, the treated PMOF/TiO₂-ReI hybrid when assisted by 0.1 M sacrificial electron donor (SED) and 3 vol% weak Brønsted acid (namely, 2,2,-trifluoroethanol (TFE)) produced persistently CO with a >99% selectivity under the visible-light irradiation condition (>500 nm). The conversion efficiency of CO₂ to CO reached up to >1,400 TON (turnover number) for a prolonged irradiation time (8 days), which appears to be the highest reported for visible-light driven CO₂ reduction systems based on combination of MOF and Re(I) molecular complex. The resultant high TON on the catalytic activity should mainly arise from fast exciton hopping transfer between adjacent porphyrin struts, which thus efficiently drives photo-electrons toward anchored Re(I) reduction center.

Poster Presentation : **INOR.P-53**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Gas sorption and capacitive properties of N-doped microporous carbon nanospheres prepared by direct carbonization of mesoporous silica nanospheres

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Department of Chemistry, Hankuk University of Foreign Studies, Korea

¹Chemistry, Hankuk University of Foreign Studies, Korea

We introduced a simple and effective direct carbonization method to synthesize N-doped microporous carbon nanospheres (MCNs). Without using additional carbon precursors, the direct carbonization of as-prepared mesoporous silica nanospheres (MSNs) containing cetylpyridinium bromide (CTPB) template led to the N-doped MCNs (SBET = 463 m² g⁻¹). From the CTPB template, N-doping process into the carbon matrix successfully occurred during the carbonization. Due to both the N-doped Lewis basic sites and uniform microporosity, the N-doped MCN was a good CO₂ adsorbent material with high CO₂ adsorption enthalpy in the low surface coverage (Q_{st} = 58.4 kJ mol⁻¹). Furthermore, the N-doped MCNs showed not only good cyclic stability during multiple CO₂ sorption but also highly selective CO₂ adsorption ability over CH₄ and H₂ at low temperature. Unique microporous features and the presence of N-dopants combined with graphitic carbon structures led to good electrochemical capacitive behavior of the N-doped MCNs. The maximum specific capacitance value of the carbon material reached up to 452.5 F g⁻¹. It also displayed great capacitance retention even after 30000 cycles.

Poster Presentation : **INOR.P-54**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Inspection of magnesium oxide as a carbon dioxide absorbent in the practical condition

Jeong-Min Lee, Jin-Su Kwak, Kang Yeong Kim, Kyung-Ryul Oh, Young-Uk Kwon*

Department of Chemistry, Sungkyunkwan University, Korea

Out of some carbon dioxide absorbents, magnesium oxide has been thought of as a practically applicable material with the help of alkaline salts in the mid-temperature range. In industrial process, 5~15 % of vapor is included in the air. This condition is thought to affect the action of magnesium oxide but has not been taken into account significantly. Herein, we set importance on figuring out how magnesium oxide is affected by vapor in real condition. For better observation, cubic shape magnesium oxide is regarded as a suitable material. Microwave-synthesis method is used to get cube magnesium oxide. We observe how cubic shape turns into depending on each cycle as the amount of vapor is fixed with 10 % portion in the furnace air. With this basis, the observation is also done when magnesium oxide is mixed with some principal promoters. Furthermore, morphology-changed magnesium oxide by vapor shows different characteristics when it reacts with carbon dioxide compared to as-synthesized cubic magnesium oxide. Details are presented in the poster.

Poster Presentation : **INOR.P-55**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of New Zeolitic Imidazolate Frameworks Using Functional Imidazoles and Structure Directing Agents

Joochan Nam, Yeongjin Kim, Seunghee Han¹, Yoojong Park¹, Soochan Lee², Wonyoung Choe^{2,*}

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In recent years, porous materials are widely used as chemical catalyst, solar cell, sensor, and so on. Among them, zeolite is one of the most famous porous materials. Zeolite has been widely used for various applications because of its stability and sorption ability. Zeolitic Imidazolate Frameworks(ZIFs) are Zeolitic MOFs(ZMOFs) that mimic zeolite, which consist of tetrahedral transition metals (Zn, Co) and various imidazoles. ZIFs share structural advantages of zeolite. However, chemical properties of ZIFs can be more easily modulated unlike zeolites. Interestingly, the number of topologies in ZIFs is relatively small compared to that for zeolites. Therefore, we have synthesized new ZIFs with new topology. In this presentation, we show that both Organic Structure-Directing Agents(OSDAs) and functional groups in ZIFs play important roles to stabilize ZIF cages.

Poster Presentation : **INOR.P-56**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Unusual Co(IV)-Oxo Structure Penetrating Oxo Wall and Its Electronic Structure Elucidated by CASSCF

**Jun-Hyeong Kim, Mahesh Sundararajan¹, Muniyandi Sankaralingam², Mu-Hyun Baik^{3,*},
Wonwoo Nam^{4,*}, Sun Hee Kim^{5,*}**

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¹*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, India*

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

⁴*Department of Chemistry, Ewha Womans University, Korea*

⁵*Western Seoul Center, Korea Basic Science Institute, Korea*

The ability to generate cobalt–oxo species is of note because of the difficulty in forming high-valent metal–oxo complexes of the late transition-metal series possessing a terminal oxo ligand in a tetragonal geometry; this difficulty is referred to as the “oxo wall”. In addition, the existence of cobalt–oxo species has garnered great interest in the communities of bioinorganic and oxidation chemistry because cobalt–oxo species have been proposed as reactive intermediates in water oxidation and C–H bond activation reactions catalyzed by cobalt-based compounds. However, cobalt–oxo species have rarely been captured in the catalytic oxidation of water and organic substrates. Furthermore, few synthetic cobalt–oxo complexes have been reported in biomimetic studies and the mechanism(s) for the oxidation reactions involving cobalt–oxo species remain unclear. Therefore, elucidation of the electronic structure of cobalt–oxo species is important for understanding cobalt–oxo chemistry, and extensive efforts have been devoted to capturing and characterizing cobalt–oxo species. However, the existence of cobalt–oxo species remains a subject of debate, with the cobalt–oxyl moiety postulated as an attractive alternative to the cobalt–oxo formulation. Thus, the electronic structure of such species needs to be clarified. Herein, we report highly complex electronic structure of a quasi-stable synthetic mononuclear nonheme cobalt–oxo species, [Co(O)(TAML)]²⁻ (TAML = tetraamido macrocyclic ligand) using Complete Active Space Self Consistent Field (CASSCF) method which is a state of the art computational tool.

Poster Presentation : **INOR.P-57**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and characterization of red emitting $K_3SiF_7:Mn^{4+}$ phosphor for white light LED application

Kangsik Choi, Younbong Park*

Department of Chemistry, Chungnam National University, Korea

Red phosphors with narrow red emission are especially interesting because they offer a wide range of color gamut and provide better rendering in LED applications such as displays and solid-state lighting. Until now, Eu^{2+} -activated silicate and nitride phosphors have been mainly studied. However, due to the emission characteristic of Eu^{2+} with a wide half-width, there is a great limitation in practical use. Since the development of the Mn^{4+} activated K_2SiF_6 phosphor with a narrow half-width, Mn^{4+} ion has been actively studied as active agents and is currently the only attraction in the LED market. We synthesized $K_3SiF_7:Mn^{4+}$ phosphor by reacting $K_2SiF_6:Mn^{4+}$ with KHF_2 under reducing atmosphere. The $K_3SiF_7:Mn^{4+}$ is crystallized with $P4/m3m$ symmetry. The luminescent properties of $K_3SiF_7:Mn^{4+}$ are almost identical to those of the $K_2SiF_6:Mn^{4+}$ phosphor, but its materials identity is distinct due to a completely different crystallographic structure. The $K_3SiF_7:Mn^{4+}$ phosphor was investigated by X-ray diffraction spectroscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, Fourier transform infrared and time-resolved photoluminescence and compared with $K_2SiF_6:Mn^{4+}$ phosphor. The $K_3SiF_7:Mn^{4+}$ phosphor can be useful in warm white LEDs and offer the possibility to develop non-rare-earth phosphors.

Poster Presentation : **INOR.P-58**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Tuning the Delayed Fluorescent Properties of ortho-carbazole- appended triarylboron compounds

Ajay Kumar, Surendran Sujith, Hanif Mubarak, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

Thermally activated delayed fluorescence (TADF) is one of the effective approaches to harvest the emissive singlet state from a triplet state via reverse intersystem crossing (RISC). Thus, by harvesting both singlet and triplet excitons, an IQE of nearly 100% can be achieved. A very small singlet-triplet energy difference (ΔE_{ST}) is required to facilitate efficient RISC. This is usually accomplished by constructing TADF emitters with a twisted donor–acceptor structure, allowing for an effective reduction in the spatial overlap between HOMO and LUMO. Recently, our group reported ortho-donor-appended triarylboron TADF emitters possessing a twisted donor–acceptor structure. In particular, the carbazole donor containing compound (CzoB) exhibited excellent efficiency in pure blue OLED. In this report, we present a series of ortho-carbazole-appended triarylboron compounds (CzRoB, Cz = 9H-carbazolyl, R = electron-withdrawing groups) where the substituents (R) were introduced to the phenylene ring of the triarylboron acceptor moiety to control LUMO level. It was shown that gradual bathochromic shifts in emission wavelength could be attained with increasing the electron-withdrawing strength of R substituent due to the stabilization of LUMO level. All of the compounds exhibit high quantum efficiency (Φ_{PL}) in oxygen-free toluene.

Poster Presentation : **INOR.P-59**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Impact of Donor and Acceptor Substitution on the Thermally Activated Delayed Fluorescence Properties in the *Ortho*-Carbazole-Appended Triarylboron Derivatives

Young Hoon Lee, Heechai Lee, Juhee Kim, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

In this work, we report on the synthesis and photophysical investigation of a series of highly efficient blue TADF materials based on the *ortho*-carbazole-linked triarylboron compounds (**1–5**) including carbazoyl unit as a donor (D) and triarylboron as an acceptor (A), respectively. The emission color of these donor-acceptor TADF emitters were finely tuned by introducing electron-donating tertiary butyl (Bu) substituents on the donor and methyl (Me) or methoxy (OMe) substituents on the acceptor units, respectively. X-ray crystal structure analysis of BuCzoB (**1**) showed a highly twisted D–A structure, leading to small singlet-triplet energy splitting. Remarkably, a high EQE value over 30% at CIE color coordinates of (0.135, 0.266) was obtained using BuCzMeoB (**2**) as the dopant. This result is ascribed to both the high quantum efficiency of **2** in the host film (93%) and the high horizontal transition dipole ratio (θ) of 0.76. Ultra-deep blue OLEDs with a record-high efficiency are also fabricated with a CzOMeOB (**5**) emitter, exhibiting an EQE of 14.9% at CIE coordinates of (0.151, 0.058).

Poster Presentation : **INOR.P-60**

Inorganic Chemistry

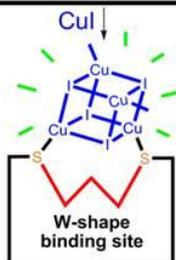
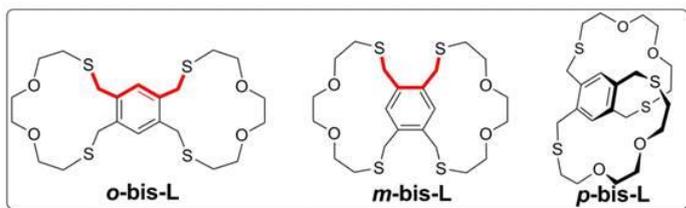
Grand Ballroom, FRI 11:00~12:30

Ligand Isomer Effect of Bis-O₂S₂-Macrocycle on Adaptive Cluster Formation and Their Homonuclear and Heteronuclear Complexes

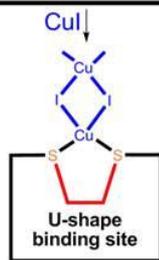
Seulgi Kim, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

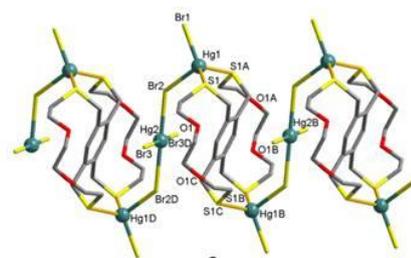
In addition to the silver(I) complexes of regioisomers (*o*-bis-L and *m*-bis-L) of bis-O₂S₂-macrocycle,¹ borderline (Pb²⁺) and soft (Hg²⁺ and Cu⁺) metal ions are employed to investigate the isomer effect.^{2,3} CuI reacts with *o*-bis-L (W-binding site) and *m*-bis-L (U-binding site) to afford 1-D CPs, [(Cu₄I₄)(*o*-bis-L)]_n (**1**) and [(Cu₂I₂)(*m*-bis-L)]_n (**2**) linked by a spacious [Cu₄I₄] cluster and a smaller [Cu₂I₂] cluster, respectively, due to the different exo-binding sites. This result illustrates the adaptive cluster formation through the binding site design. Lead(II) perchlorate afforded a 1-D CP {[Pb₂(*o*-bis-L)(ClO₄)₂(ClO₄)₂]}_n (**3**) and a discrete complex [Pb₂(*m*-bis-L)(CH₃CN)₂(H₂O)₂(ClO₄)₂(ClO₄)₂] (**4**), in which both are based on the endocyclic binuclear complexes due to the oxophilicity of lead(II). Meanwhile, mercury(II) halides showed an endocyclic dinuclear complex [Hg₂(*o*-bis-L)I₂][Hg₃I₈] (**5**) and an exocyclic 1-D CP [Hg₃(*m*-bis-L)Br₆]_n (**6**) because of the different S...S separation in the two isomers. A mixture of mercury(II) iodide and copper(I) iodide afforded a heterometallic 1-D CP [Cu₂Hg₂(*m*-bis-L)(Cu₂I₂)(CH₃CN)₂I₆]_n (**7**) in which the exocyclic dicopper(I) complex units are linked by -Hg-Cu₂I₄-Hg- segments to form a zigzag chain. **References**[1] Siewe, A. D.; Kim, J.-Y.; Kim, S.; Park, I.-H.; Lee, S. S. *Inorg. Chem.* **2014**, *53*, 393.[2] Kim, S.; Siewe, A. D.; Lee, E.; Ju, H.; Park, I.-H.; Park, K.-M.; Ikeda, M.; Habata, Y.; Lee, S. S. *Inorg. Chem.* **2016**, *55*, 2018.[3] Kim, S.; Siewe, A. D.; Lee, E.; Ju, H.; Park, I.-H.; Jung, J. H.; Habata, Y.; Lee, S. S. *Cryst Growth Des.* **2018**, *18*, 2424.



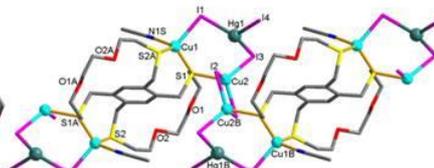
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Poster Presentation : **INOR.P-61**

Inorganic Chemistry

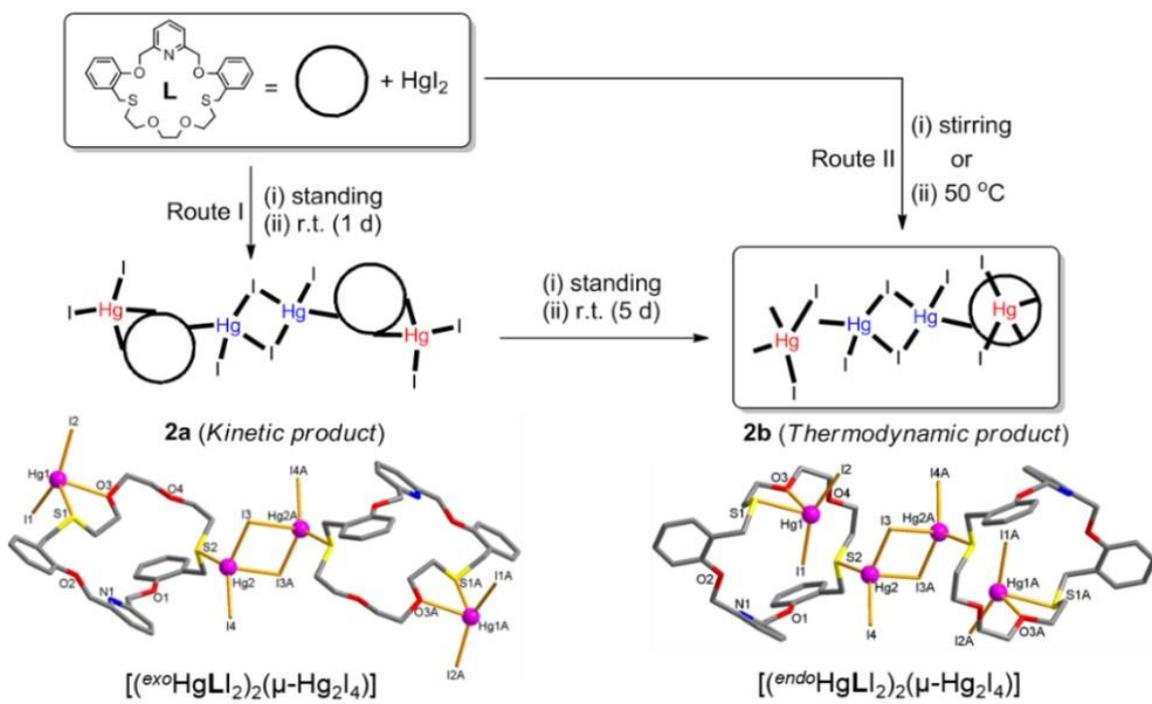
Grand Ballroom, FRI 11:00~12:30

A Ditopic 23-Membered NO₄S₂-Macrocyclic and Its Soft Metal Complexes as Kinetic and Thermodynamic Products

Mingyeong Shin, Huiyeong Ju, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

A ditopic 23-membered NO₄S₂-macrocyclic (**L**) incorporating rigid and flexible binding sites and its soft metal complexes exhibiting different stoichiometries and coordination modes were synthesized and structurally characterized. First, silver(I) perchlorate reacts with **L** to afford an endocyclic mononuclear complex [Ag(**L**)]ClO₄ (**1**) in which the silver(I) ion locates at the rigid binding site of the macrocyclic cavity adopting a penta-coordinated SP geometry. NMR titration for the corresponding system also shows of an 1:1 (metal-to-ligand) stoichiometry in solution. Interestingly, reaction of **L** with HgI₂ led to the isolation of two tetranuclear bis(macrocyclic) complexes, [(^{exo}Hg**L**I₂)₂(μ-Hg₂I₄)] (**2a**) and [(^{endo}Hg**L**I₂)₂(μ-Hg₂I₄)] (**2b**), as a kinetic and a thermodynamic product, respectively (*see below*). In both products, two exocyclic (**2a**) and two endocyclic (**2b**) mercury(II) complex units are linked by tetraiododimercury(II) core, (μ-Hg₂I₄), to give a 4:2 stoichiometry. The reaction of **L** with copper(I) chloride yielded a greenish complex of the formula [Cu^I(**L**)Cl₂]·CH₃CN (**3**), exhibiting the oxidation of copper(I) to copper(II). When a mixture of CdI₂ and HgI₂ was used in the reaction with **L**, a discrete type complex with two separated parts of the formula [Cd(**L**)I]₂[Hg₂I₆] (**4**) was isolated.



Poster Presentation : INOR.P-62

Inorganic Chemistry

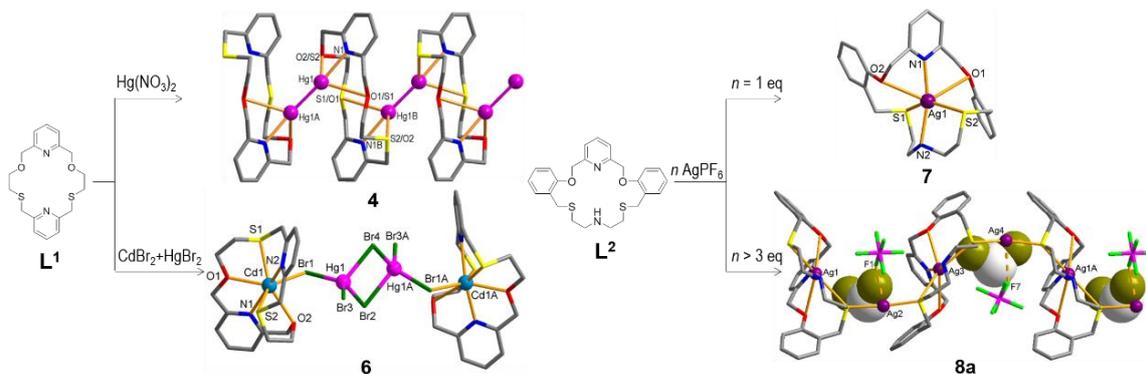
Grand Ballroom, FRI 11:00~12:30

Ditopic N₂O₂S₂-Macrocycles Incorporating Hard Base and Soft Base Parts Simultaneously and Their Supramolecular Complexes

Sujin Seo, Eunji Lee , Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

As ditopic host system incorporating hard base and soft base domains, an 18-membered (**L**¹ and a 20-membered (**L**²)²⁻⁴ N₂O₂S₂-macrocycles and their supramolecular complexes are reported. The reactions of ZnBr₂ and CdBr₂ with **L**¹ afforded mononuclear complexes [Zn(**L**¹)] [ZnBr₄] (**1**) and [Cd(**L**¹)Br₂] (**2**), respectively. When HgBr₂ was used, a dinuclear complex [Hg₂(**L**¹)Br₄] (**3**) was obtained. While, Hg(NO₃)₂ gave a 1-D CP {[Hg₂(**L**¹)](NO₃)₂]_n (**4**, see below) as a first example of the infinite macrocyclic mercury(I) complex. The reaction of a mixture of ZnBr₂ and CdBr₂ afforded two solubility-dependent Cd(II) complexes (**2** and **5**) including a half dumbbell-type complex [Cd(**L**¹)(μ-Br)(CdBr₃)] (**5**). Interestingly, one-pot reaction of a mixture of CdBr₂ and HgBr₂ afforded a dumbbell-type heterometallic product [(Cd**L**¹)₂(μ-Hg₂Br₆)](Hg₂Br₆) (**6**, see below). In the equimolar reaction of **L**², AgPF₆ afforded a typical endocyclic complex [Ag(**L**²)](PF₆) (**7**). However, the use of three equivalents or above amount of AgPF₆, gave an endo/exocyclic 1-D CP {[Ag₄(**L**²)₂](PF₆)₄·2CH₂Cl₂]_n (**8a**, see below). Upon removal of the lattice dichloromethane molecules in the ambient condition, conversion of the coordination geometry of the exo-Ag atom from linear (**8a**) to trigonal plane (**8b**, {[Ag₄(**L**²)₂](PF₆)₂](PF₆)₂]_n) as well as sliding of the 1-D chains were observed in an SCSC manner.



Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Molecular-Level Studies of Amyloid- β and Proteins: Interactions with and without Metal Ions and Aggregation

Hyuck Jin Lee, Tae Su Choi¹, Masha G. Savelieff², Megan Brunjes Brophy³, Toshiki G. Nakashige³, Elizabeth M. Nolan^{3,*}, Hugh I. Kim^{1,*}, Mi Hee Lim^{4,*}

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Deposition of misfolded protein aggregates, such as senile plaques composed of amyloid- β (A β) aggregates, is a characteristic feature of Alzheimer's disease (AD).^{1,2} Due to this hallmark of the disease and toxicity associated with A β aggregates, previous studies have focused on understanding and modulating A β aggregation pathways. In the brain, the aggregation of A β could be affected by (i) metal ions, such as Zn(II) and Cu(II), which are observed to bind to A β and accelerate its aggregation; (ii) proteins which could interact with A β [*e.g.*, human serum albumin (HSA; the most abundant plasma protein)] or (iii) be overexpressed and possibly co-localized with A β aggregates in the AD-affected brain [*e.g.*, S100A8 and S100A9 which exist as heterodimeric form of S100A8/S100A9, called calprotectin (CP)]. HSA and S100A9 have been suggested to suppress and facilitate the aggregation of metal-free A β , respectively;^{3,4} however, the information on their interactions with metal-free A β has been still limited. In addition, although HSA and CP can interact with metal ions, their direct interaction and influence on the aggregation pathways and toxicity of metal-associated A β have been rarely reported. In this presentation, we will present the ability of HSA and CP to modulate the aggregation of A β with and without metal ions possibly through direct interaction with A β . HSA and CP could form complexes with A β peptides, alter their aggregation pathways, and affect the toxicity induced by metal-free and metal-bound A β to different degrees. Our overall investigations demonstrate a potential network among A β , protein(s), and metal ions related to the pathogenesis of AD.^{5,6} References 1. Savelieff, M. G.; Nam, G.; Kang, J.; Lee, H. J.; Lee, M.; Lim, M. H. *Chem. Rev.* 2018, DOI: 10.1021/acs.chemrev.8b00138. 2. Lee, S. J. C.; Nam, E.; Lee, H. J.;

Savelieff, M. G.; Lim, M. H. *Chem. Soc. Rev.* 2017, 46, 310-323.3.Milojevic, J.; Costa, M.; Ortiz, A. M.; Jorquera, J. I.; Melacini, G. J. *Alzheimers Dis.* 2014, 38, 753-765.4.Zhang, C.; Liu, Y.; Gilthorpe, J.; van der Maarel, J. R. C. *PLoS One*, 2012, 7, e32953.5.Lee, H. J.;§ Savelieff, M. G.;§ Kang, J.; Brophy, M. B.; Nakashige, T. G.; Lee, S. J. C.; Nolan, E. M.; Lim, M. H. *Metallomics* 2018, 10, 1116-1127 (§co-first authorship).6.Choi, T. S.;§ Lee, H. J.;§ Han, J. Y.; Lim, M. H.; Kim, H. I. *J. Am. Chem. Soc.* 2017, 139, 15437-15445 (§co-first authorship).

Poster Presentation : **INOR.P-64**

Inorganic Chemistry

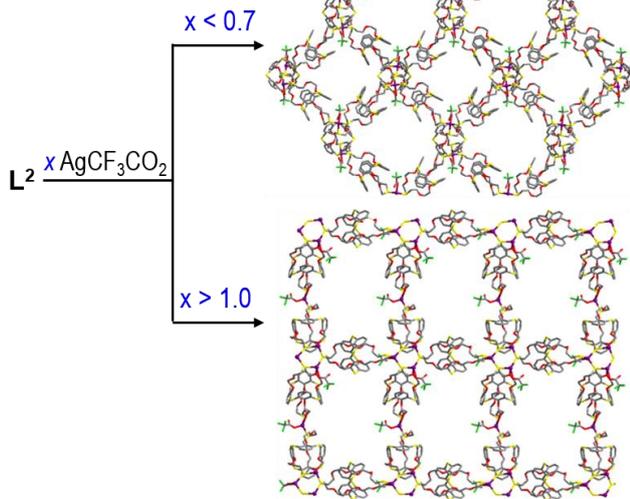
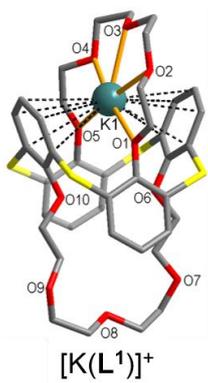
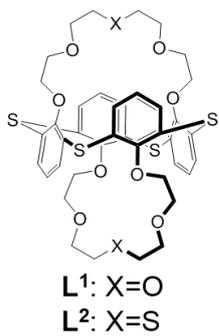
Grand Ballroom, FRI 11:00~12:30

Supramolecular Complexes of Ditopic Thiacalix[4]-*bis*-(thia)crowns

Huiyeong Ju, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

Thiacalix[4]-*bis*-crown (**L**¹) and thiacalix[4]-*bis*-thiacrown (**L**²) were employed as building blocks for supramolecular complexes. Reaction of **L**¹ with KClO₄ afforded an endocyclic dipotassium(I) complex [K₂(**L**¹)](ClO₄)₂·CH₃CN (**1**). Its monopotassium(I) complex [K(**L**¹)] [Pt(tht)Cl₅] (**2**, tht = tetrahydrothiophene) was also isolated from the mixed salts as a first example of symmetrical calix[4]-*bis*-crowns (*see below*). In the silver(I) complexations, anion-dependent exocyclic silver(I) coordination polymers (CPs) were isolated (**3**: perchlorate and **4**: nitrate). When silver(I) perchlorate was used, for example, a double-stranded 1D CP {[Ag₂(**L**¹)(ClO₄)₂]CH₂Cl₂}_n (**3**) was obtained, while silver(I) nitrate afforded {[Ag₂(**L**¹)(NO₃)₂]CH₃OH}_n (**4**) with a brick-wall type 2D CP structure. Unlike **L**¹, silver(I) complexations with **L**² afforded the mole ratio dependent products. Below 0.7 equiv of AgCF₃CO₂, 2D CP {[Ag₂(**L**²)(CF₃CO₂)₂]6CHCl₃}_n (**5**) was isolated. Notably, the use of 1.0 equiv or above amount of AgCF₃CO₂ gave a different 2D CP, {[Ag₄(**L**²)(CF₃CO₂)₄]·CHCl₃·toluene·CH₃OH}_n (**6**). To monitor the mole ratio dependency, the PXRD analysis has been applied.



Poster Presentation : **INOR.P-65**

Inorganic Chemistry

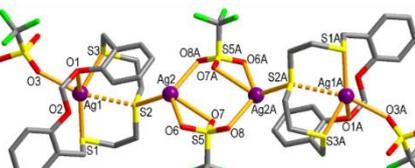
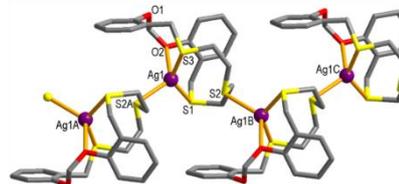
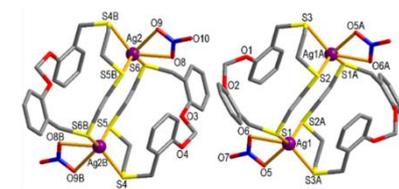
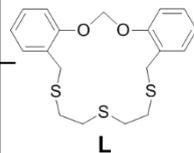
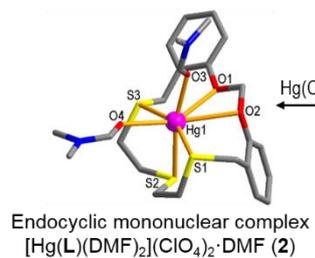
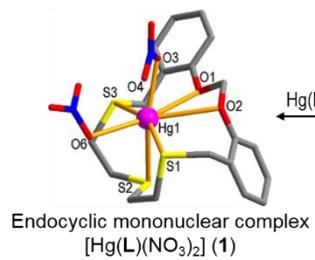
Grand Ballroom, FRI 11:00~12:30

Anion-Controlled Topologies and Coordination Modes of Soft Metal Complexes with an O₂S₃-Macrocyclic

Yoonji Kim, Huiyeong Ju, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

An O₂S₃-macrocyclic (**L**) was employed as a soft base ligating system. Five soft metal complexes (**1-5**) of **L** were prepared and structurally characterized. Both mercury(II) complexes with nitrate [Hg(**L**)(NO₃)₂] (**1**) and perchlorate [Hg(**L**)(DMF)₂](ClO₄)₂·DMF (**2**) anions show a typical endocyclic structure. The silver(I) complexation is more challenging on the role of anions. For example, nitrate afforded a cyclic dimer complex [Ag₂(**L**)₂(NO₃)₂] (**3**) in which two exocyclic silver(I) link two facing macrocycles to give a metallacycle. While hexafluorophosphate gave a 1-D coordination polymer {[Ag(**L**)]PF₆}_n (**4**). In **4**, macrocycles are linked by silver(I) in an **L**-Ag-**L**-Ag pattern. Interestingly, the reaction of **L** with AgCF₃SO₃ led to the isolation of a tetranuclear bis(macrocycle) complex, {[^{endo}Ag(**L**)(CF₃SO₃)]₂[μ-^{exo}Ag₂(CF₃SO₃)₂]} (**5**), dominated by the coordination modes of **L** toward two types of mercury(II) centers. For instance, two endocyclic complex units, ^{endo}Ag₂(**L**)₂(CF₃SO₃)₂, are linked by exocyclic metallacycle [μ-^{exo}Ag₂(CF₃SO₃)₂] core to give a 4:2 (metal-to-ligand) stoichiometry.



Poster Presentation : **INOR.P-66**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Time-dependents self-assembly. Transformation of Cyclophane-Type 1D Linked Ring into Simple Linked Ring

Dongwon Kim, Ok-Sang Jung*, SeongHyeon Park

Department of Chemistry, Pusan National University, Korea

Self-assembly of AgX (X = CF₃SO₃⁻ and PF₆⁻) with 1,3,5-tris(nicotinoyloxy-methyl)benzene (L) initially produces a cyclophane-type 30-membered macrocyclic linked 1D network with composition of Ag(I) and L of 3:2 irrespective of anion and solvent. After 20 days, The 1D networks of [Ag₉(CF₃SO₃)₄L₆(C₄H₈O)₅](CF₃SO₃)₅ and [Ag₃L₂(C₄H₈O)₂](PF₆)₃ are changed the crystalline products in the mother liquor are changed to 16-membered macrocyclic linked 1D with composition of Ag(I) and L of 1:1 ratio into [AgL(CF₃SO₃)] and [AgL](PF₆). All crystal structures show significantly the metalophilicity of two anions CF₃SO₃⁻ and PF₆⁻.

Poster Presentation : **INOR.P-67**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cage Effect on Oxidation via Pd₂L₄ Prolate Spheroid

EunSoo Yi, Ok-Sang Jung*, Hyejin Oh

Department of Chemistry, Pusan National University, Korea

Self-assembly of PdX₂ (X⁻ = NO₃⁻, BF₄⁻, and CF₃SO₃⁻) with 2,6-bis(4'-nicotinamidophenoxy)naphthalene (L) forms a series of [Pd₂L₄]X₄ prolate spheroids. The O donors of two Me₂SO molecules within the prolate spheroid cage are oriented toward Pd(II) metal centers. In the presence of H₂O₂, the nestled Me₂SO within cage is efficiently oxidized to Me₂SO₂ at room temperature. The cage effect will be discussed.

Poster Presentation : **INOR.P-68**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Catalytic Effects of Bimetallic Copper(II) Cases

Lingling Yang, Jyoti Ramesh Jadhav, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of $\text{Cu}(\text{OTf})_2$ with a new N,N',N'' -((benzene-1,3,5-triyltris(oxy))tris(benzene-2,1-diyl))trinicotinamide ligand (L) in a mixed solution of acetone and chloroform gives rise to crystals of cyclodimeric $[\text{Cu}_2\text{L}_2(\text{OTf})_3(\text{acetone})(\text{H}_2\text{O})_2] \cdot 3\text{CHCl}_3 \cdot (\text{OTf}) \cdot \text{H}_2\text{O}$. When the crystal was recrystallized in a mixture of tetrahydrofuran and chloroform, new blue crystal, $[\text{Cu}_2\text{L}_2(\text{OTf})_3(\text{H}_2\text{O})_3] \cdot 3\text{CHCl}_3 \cdot \text{THF} \cdot (\text{OTf}) \cdot \text{H}_2\text{O}$, was obtained after 4 days. Their skeletal structures are originally similar except for coordinated acetone and H_2O molecules, respectively. These crystals have been employed as catalysts for 3,5-di-*tert*-butylcatechol oxidation, showing significant different catalytic effects between two species.

Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Recognition of Cyclodimeric Zn(II) Complexes

SooMin Hyun, Ah Reum Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of ZnI_2 with di(isoquinolin-5-yl)isophthalate (L) as a new bidentate *N*-donor gives rise to a discrete crown-shaped M_2L_2 architecture, $[Zn_2I_4L_2] \cdot 4CH_3CN \cdot THF$. These cyclodimers constitute, a characteristically eclipsed molecular array, resulting in the formation of channels. The metalocyclodimer effectively stabilizes/recognizes a combination aggregate of unstable CH_2I_2 and benzene molecules. UV-irradiation 254 nm on $[Zn_2I_4L_2] \cdot 4CH_3CN \cdot THF$ crystal has been attempted. Their photoreactivity will be presented.

Poster Presentation : **INOR.P-70**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Organization of Various Aromatics Guests within Nano-channel MOFs

Daseul Lee, Sarada Ganguri, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of Ag(I) ions with *N,N,N'*-tris(2-(pyridin-4-yl)ethyl)-1,3,5-benzenetricarboxamide (L) produces unique 2D metal-organic frameworks (MOFs). The assembly of each 2D MOF via $\pi\cdots\pi$ stacking (4.561 Å) forms 3D MOFs consisting of nano-channels (32.234 X 17.713 Å²), resulting in nano-channel hydrophobicity. The hydrophobic nano-channel effectively adsorbs a wide range of fused hydrocarbons (FAHs) in the monomeric or dimeric mode, which makes it potentially highly useful as an energy-transfer material.

Poster Presentation : **INOR.P-71**

Inorganic Chemistry

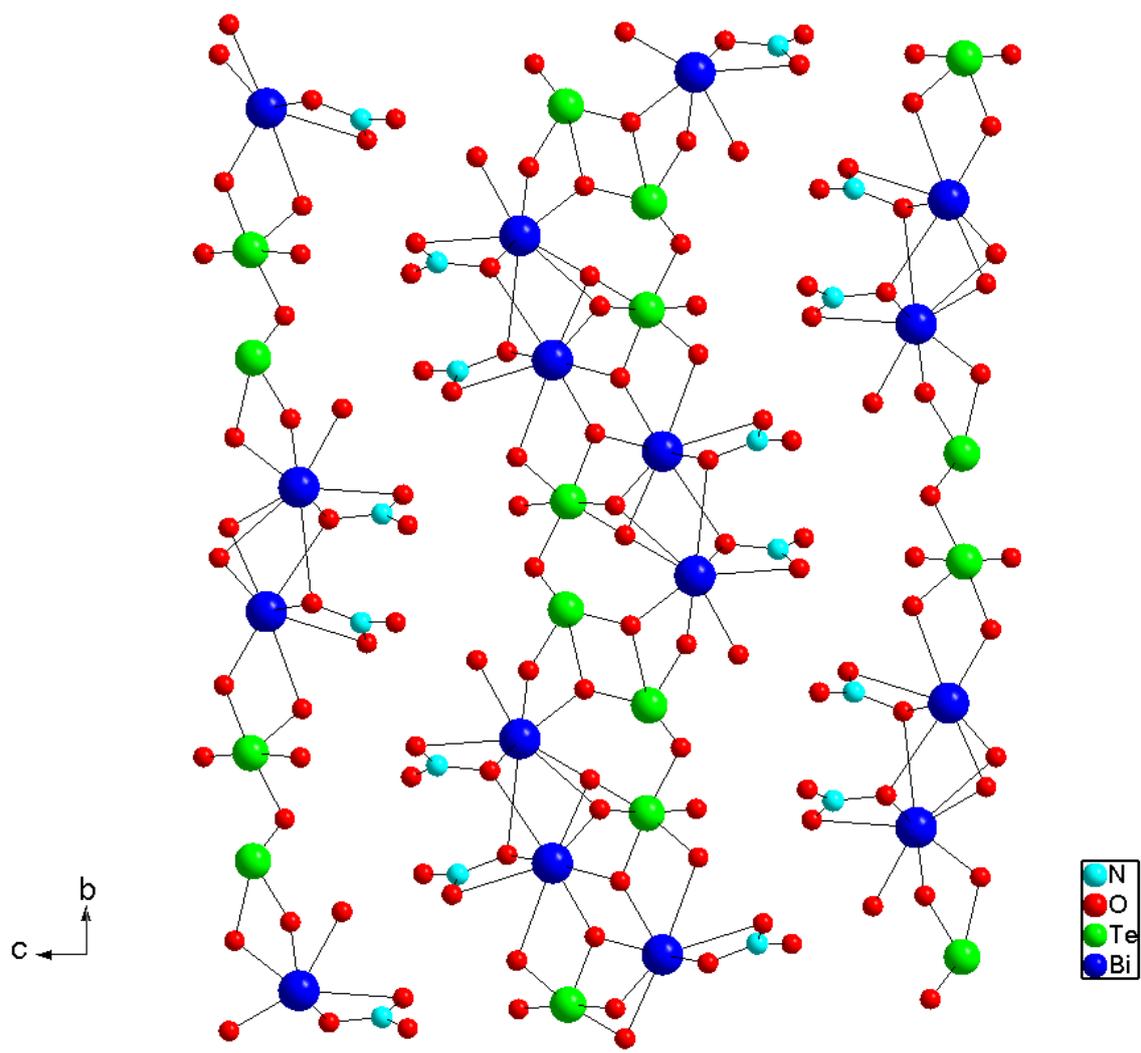
Grand Ballroom, FRI 11:00~12:30

Synthesis and characterization of a noncentrosymmetric layered material $\text{Bi}_2\text{Te}^{\text{IV}}\text{Te}^{\text{VI}}\text{O}_6(\text{NO}_3)_2(\text{H}_2\text{O})(\text{OH})_2$

So Yon Lee, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Materials crystallizing in noncentrosymmetric (NCS) structures may show certain properties such as pyroelectricity, piezoelectricity, ferroelectricity, and nonlinear optical properties. To achieve a macroscopic NCS structure, bismuth, tellurium, and NO_3^- were used in the synthesis as constituents. Since the lone pairs on Bi^{3+} and Te^{4+} cations are stereochemically active, they can exhibit asymmetric coordination environment. The π -conjugated electron in the NO_3^- group can also facilitate the nonlinear optical property. The hydrothermally synthesized material reveals a layered nonpolar structure with a weak hydrogen bond interaction. The compound crystallizes in the orthorhombic space group, $P2_12_12_1$. Two types of existing telluriums, Te^{4+} and Te^{6+} show see-saw and octahedral coordination environment with oxide ligands, respectively. Bi^{3+} cations are linked to oxygen atoms and form BiO_9 and BiO_{10} polyhedra. NO_3^- is connected to the bismuth atoms. Powder second-harmonic generation (SHG) measurements indicate that the NCS material has a SHG efficiency of 20 times that of $\alpha\text{-SiO}_2$. Further experiments were performed to exfoliate the layers of the material. By adding diluted hydrazine to the sonicated crystals, exfoliated products were obtained, which were characterized by X-ray diffraction and SEM.



Poster Presentation : **INOR.P-72**

Inorganic Chemistry

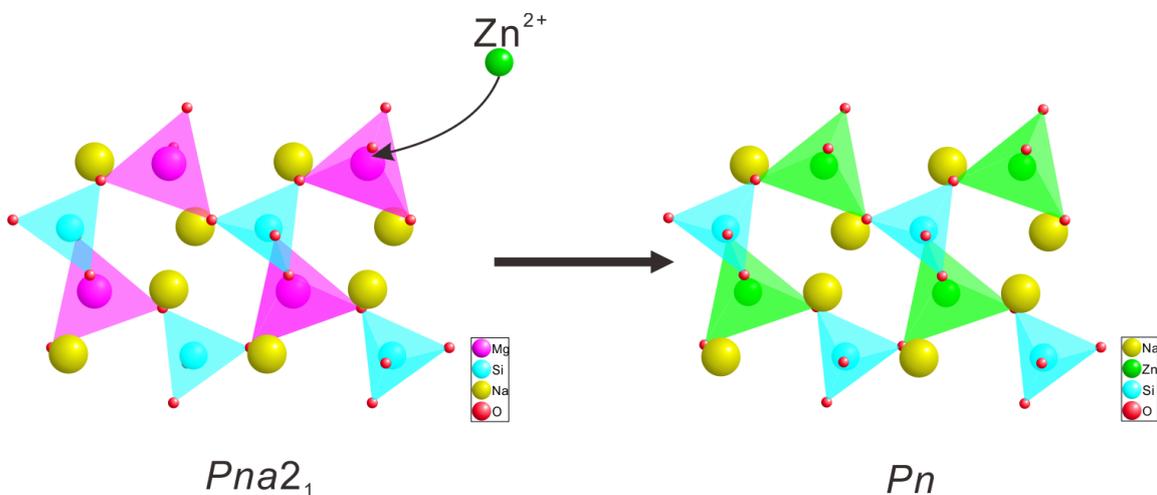
Grand Ballroom, FRI 11:00~12:30

Solid State Synthesis and Second Harmonic Generation Properties of $\text{Na}_2\text{Mg}_{1-x}\text{Zn}_x\text{SiO}_4$ ($x = 0-1.0$) Solid Solutions

Hyeshin Lee, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

A series of sodium metal silicate solid solutions, $\text{Na}_2\text{Mg}_{1-x}\text{Zn}_x\text{SiO}_4$ ($x = 0-1.0$) has been successfully synthesized through high temperature solid state reactions. While the space group of a model compound, $\text{Na}_2\text{MgSiO}_4$ is $Pna2_1$ (Orthorhombic), $\text{Na}_2\text{ZnSiO}_4$ crystallizes in Pn (Monoclinic). Na_2MSiO_4 ($M = \text{Mg, Zn}$) consists of SiO_4 , MO_4 tetrahedral and sodium cations. The two original compounds reveal similar structures and both materials are crystallizing in noncentrosymmetric space groups. Furthermore, the solid solutions, $\text{Na}_2\text{M}_{1-x}\text{Zn}_x\text{SiO}_4$ ($x = 0.2, 0.4, 0.6, 0.8$), crystallize in either $Pna2_1$ or Pn . The crystal structures of the reported solid solutions were determined by powder X-ray diffraction. Phase transition depending on the amount of transition metal cations has been studied by the diffraction method. In addition, the effect of polarization of d^{10} transition metal cations on the second-harmonic generation properties of the solid solutions has been also examined.



Poster Presentation : **INOR.P-73**

Inorganic Chemistry

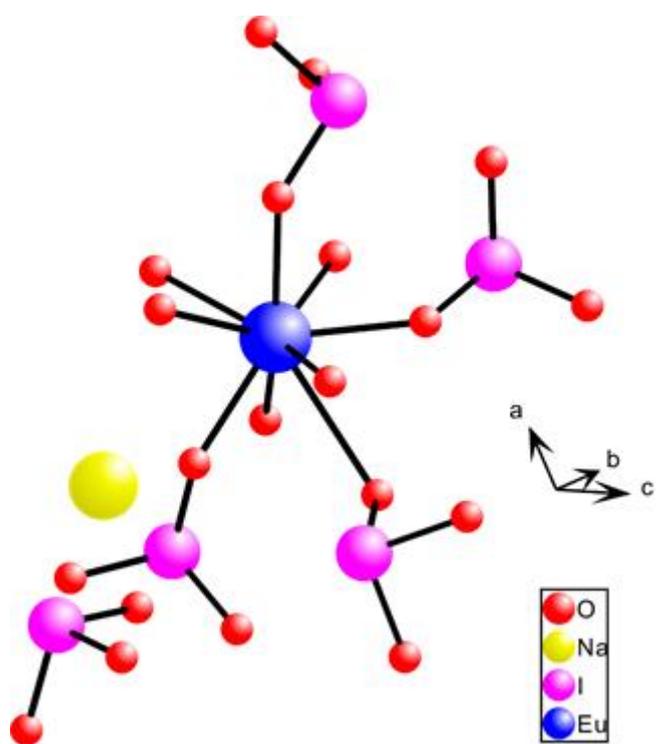
Grand Ballroom, FRI 11:00~12:30

Hydrothermal synthesis, structure, and characterization of a noncentrosymmetric europium iodate

Hyerin Song, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Metal iodates containing IO_3 polyhedra in asymmetric coordination environment due to the stereochemically active lone pairs can be used as useful optical materials in a wide transparent spectral range. In this research, we have synthesized a new europium iodate by a hydrothermal reaction using Na_2CO_3 , $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, HIO_3 , and water as reagents. The crystal structure of the europium iodate compound was determined using single crystal X-ray diffraction. The title compound crystallizes in the rhombohedral space group, $R3c$ (No. 146), and consists of EuO_8 , IO_3 , and Na^+ ions. A complete characterization including the energy dispersive X-ray spectroscopy (EDS), infrared, UV-vis diffuse-reflectance spectroscopy, thermogravimetric analysis (TGA) and second harmonic generation (SHG) will be presented.



Poster Presentation : **INOR.P-74**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Structure of Three Polyoxomolybdates with Peroxo ligands

Jiyeon Hwang, Kang Min Ok^{1,*}

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Three novel polyoxomolybdates with peroxo ligands, $\text{Rb}_5[\text{Na}(\text{H}_2\text{O})_5][\text{Mo}_7(\text{O}_2)_2\text{O}_{22}]\cdot\text{H}_2\text{O}$ (**Rb-1**), $\text{Cs}_5[\text{Na}(\text{H}_2\text{O})_5][\text{Mo}_7(\text{O}_2)\text{O}_{23}]\cdot\text{H}_2\text{O}$ (**Cs-1**) and $\text{Cs}_4[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]\cdot\text{H}_2\text{O}$ (**Cs-2**) have been synthesized through a slow evaporation method. The title compounds were characterized using powder X-ray diffraction and single crystal X-ray diffraction. All compounds crystallize in the triclinic space group, *P*-1. Both **Rb-1** and **Cs-1** consist of Rb^+ or Cs^+ cations, $\text{Na}(\text{H}_2\text{O})_5$ and polyoxoanion clusters, $[\text{Mo}_7(\text{O}_2)_2\text{O}_{22}]^{6-}$ (Figure 1) and $[\text{Mo}_7(\text{O}_2)\text{O}_{23}]^{6-}$ (Figure 2), while **Cs-2** consists of Cs^+ cations and $[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]^{4-}$ (Figure 3) polyoxoanions. All the reported compounds contain peroxo ligand and the oxidation states of the molybdenum are +6. An interesting phase transition from **Cs-1** to **Cs-2** was monitored during the evaporation of Cs-containing solutions. It is considered that **Cs-1** is a metastable compound, whereas **Cs-2** is thermodynamically stable product. Further studies to elucidate the transition mechanism of the reported compounds are ongoing.

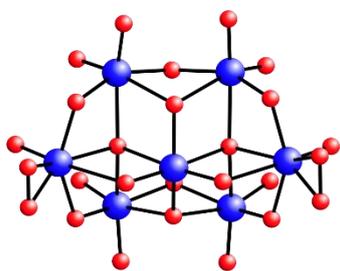


Figure 1. $[\text{Mo}_7(\text{O}_2)_2\text{O}_{22}]^{6-}$ (**Rb-1**)

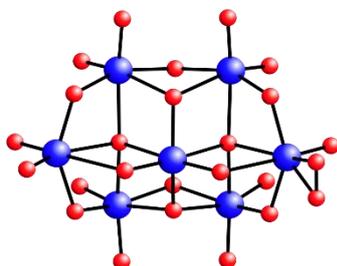


Figure 2. $[\text{Mo}_7(\text{O}_2)\text{O}_{23}]^{6-}$ (**Cs-1**)

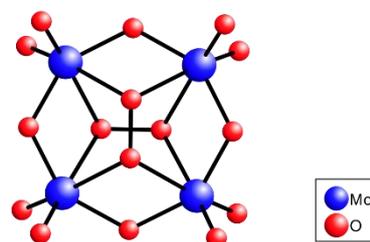


Figure 3. $[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]^{4-}$ (**Cs-2**)



Poster Presentation : **INOR.P-75**

Inorganic Chemistry

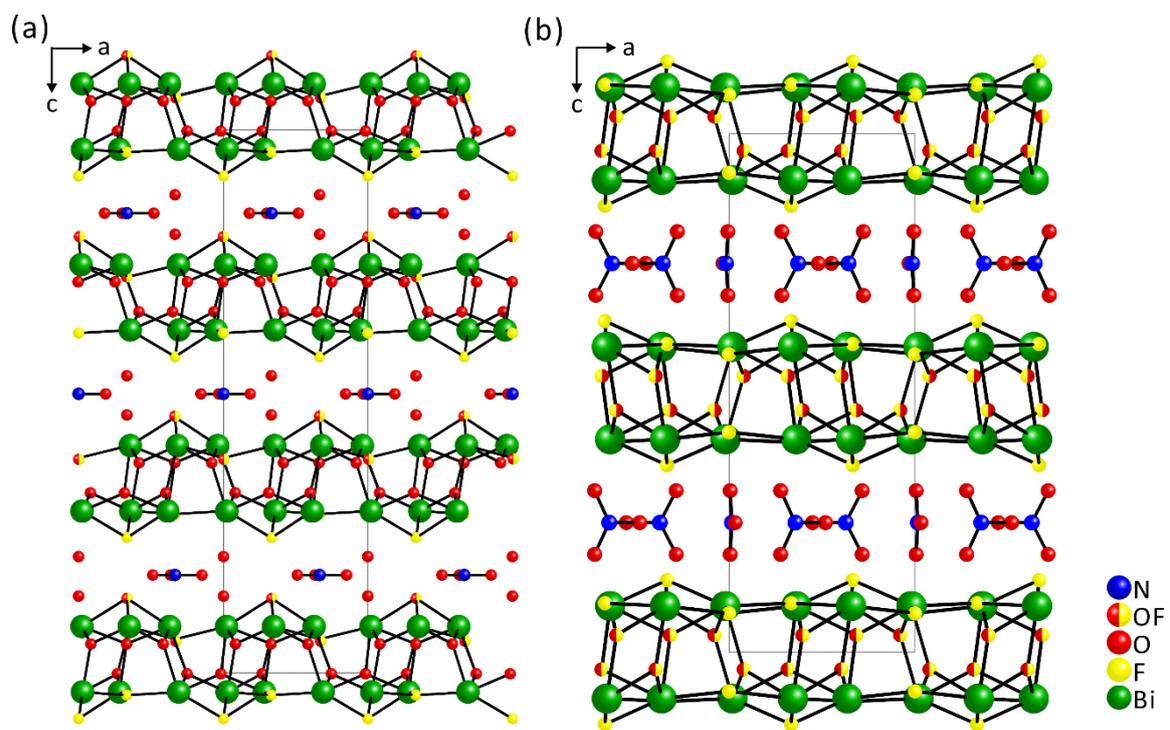
Grand Ballroom, FRI 11:00~12:30

Hydrothermal synthesis, crystal structure, and second-harmonic generating (SHG) properties of two layered bismuth oxyfluoride nitrate materials.

EunJeong Cho, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

New layered noncentrosymmetric (NCS) and centrosymmetric (CS) bismuth oxyfluoride-nitrate materials were synthesized by hydrothermal reactions. The crystal structures were determined by powder and single-crystal X-ray diffraction. The NCS material crystallizes in the trigonal space group, $R\bar{3}$ (No. 146). The CS material crystallizes in the hexagonal space group, $P6_3/m$ (No. 176). The powder second harmonic generation (SHG) measurements indicate the compound crystallizing in the NCS structure is phase-matchable (Type I) and exhibits a strong SHG efficiency of about 90 times that of α -SiO₂. Infrared and UV-vis diffuse-reflectance spectroscopy, energy dispersive X-ray spectroscopy (EDS), thermogravimetric analysis (TGA), and local dipole moment calculations are also presented.



Poster Presentation : **INOR.P-76**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Solvothermal Synthesis, Crystal Structures, and Characterization of Two New Metal-Organic Coordination Polymers, [(TC)₆Zn₃(bipy)] and [(TC)₆Co₃(bipy)]

Jungjoo Kim, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Two new metal organic coordination polymers, [(TC)₆Zn₃(bipy)] (1) and [(TC)₆Co₃(bipy)] (2) (bipy = 4,4'-bipyridine and TC = 3-thiophenecarboxylate) were successfully synthesized by solvothermal reactions. The two coordination polymers were crystallized in the triclinic space group, *P*-1 (No. 2), which was determined by single crystal X-ray diffraction. The title compounds are isostructural each other and reveal infinite chain structures consisting of MO₆ octahedra, MO₄N trigonal bipyramidal, TC, and bipy ligands (M = Zn²⁺ or Co²⁺). M²⁺ cations are coordinated by TC ligands and form M₃O₁₂N₂ trimers. The trimers are very similar to the peddle wheel structure. The reported coordination polymers were characterized by powder X-ray diffraction, IR spectroscopy, thermogravimetric analysis, elemental analysis, and UV-Vis diffuse reflectance spectrum. Photoluminescence and direct-current magnetic susceptibility are also presented.

Poster Presentation : **INOR.P-77**

Inorganic Chemistry

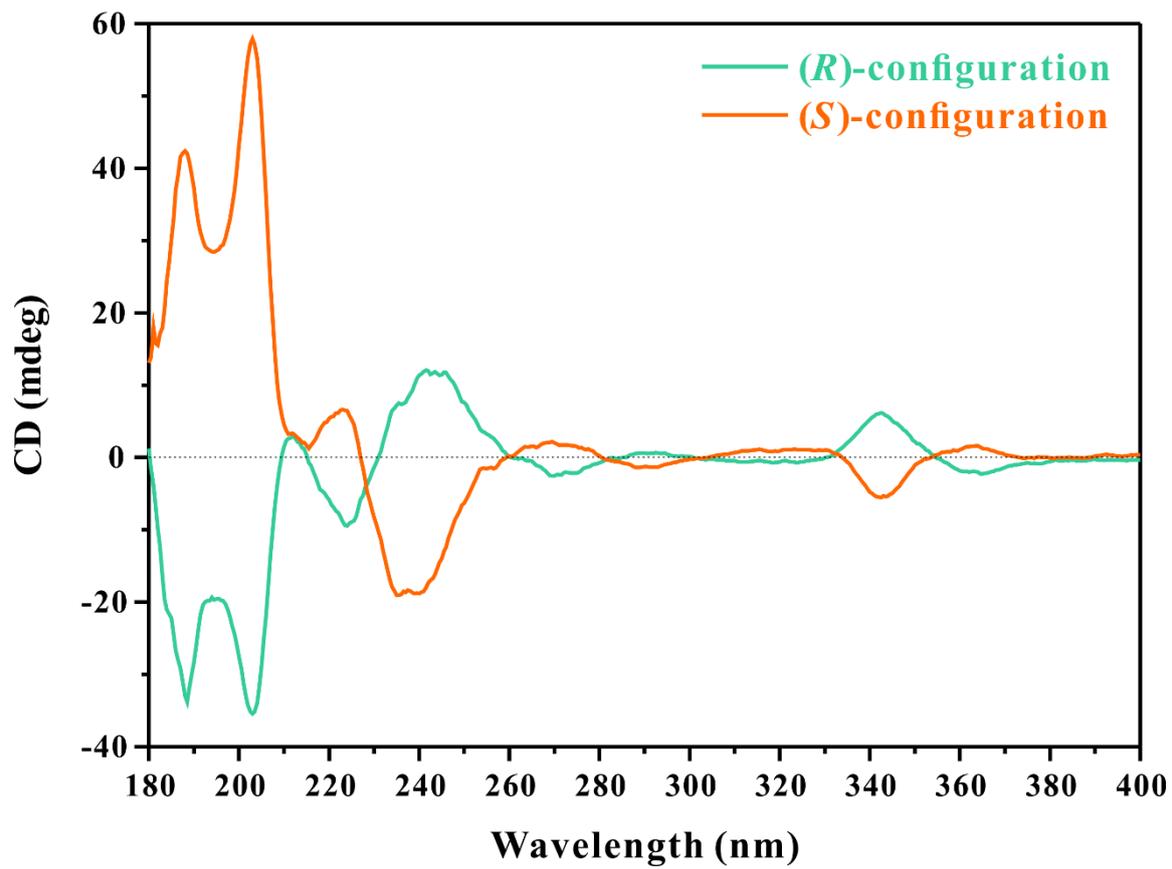
Grand Ballroom, FRI 11:00~12:30

A Novel Chiral Organic-Inorganic Hybrid Bismuth Bromide

TaeHwan Moon, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

In recent years, organic-inorganic hybrid perovskites such as methylammonium lead halides (MAPbI₃), which can increase the efficiency of solar cells, have been widely investigated owing to their low costs and simple processes of production. A new hybrid chiral material composed of (*R*)/(*S*)-1-phenylethylamine and bismuth bromide was synthesized using a mild solution chemistry method. Single crystal X-ray diffraction analysis indicates that both (*R*)- and (*S*)-configuration materials were successfully synthesized. To find applicability to photovoltaic or optoelectronic devices, the newly synthesized chiral materials were uniformly deposited on glass substrates by the spin-coating method. Powder X-ray diffraction analysis on the chiral thin films indicate that both (*R*)- and (*S*)-configuration materials reveal a strong preferred orientation along the crystallographic *a*-axis. We also determined the chirality of thin films through solid state circular dichroism analysis. Infrared spectra, UV-vis reflectance spectra, and second harmonic generation measurements were also performed for both polycrystalline as well as thin film samples.



Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of Ruthenium Nitrosyl Complex with Quinoline Derivative Ligand

Eun su Chae, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Nitric oxide (NO), which can control many biological functions, is produced from L-arginine by nitric oxide synthases (NOSs) in mammals. Three isoenzymes of NOS, endothelial NOS (eNOS), neuronal NOS (nNOS), and inducible NOS (iNOS), have been classified according to the locations where the enzymes are expressed. Among the isoenzymes, iNOS has an ability to destroy tumor cells by high level of NO production. This has increased the researches looking for iNOS-like complexes, which are capable of releasing a large amount of NO by specific chemical or physical stimuli. We have been developing ruthenium nitrosyl complexes which can release NO by visible light for photodynamic therapy (PDT). In this poster, we present the synthesis and photoreactivity of a novel ruthenium nitrosyl complex with tetradentate quinoline type ligand.

Poster Presentation : **INOR.P-79**

Inorganic Chemistry

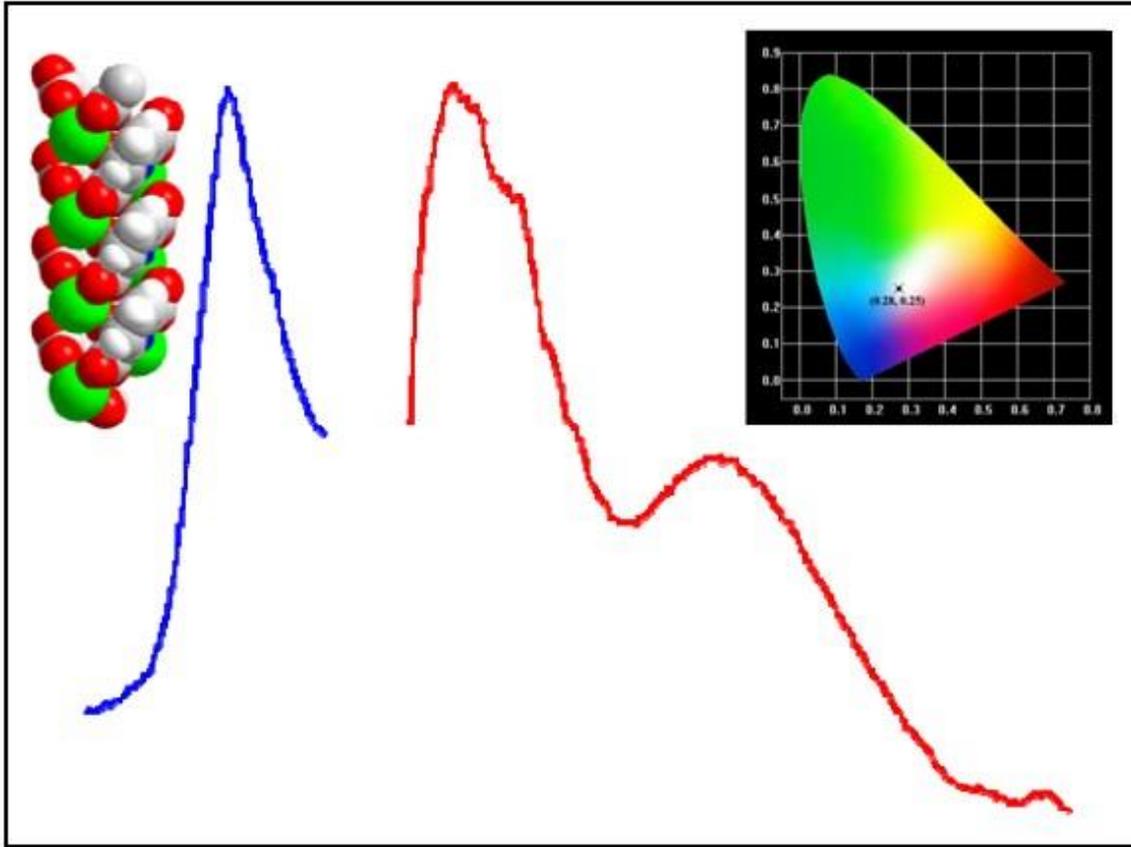
Grand Ballroom, FRI 11:00~12:30

Pb[NC₅H₃(CO₂)₂]: A highly thermostable white light emitting single component coordination compound

Haixin Qi, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

A lead-based coordination compound, Pb[NC₅H₃(CO₂)₂] with a pseudo-2D topology has been hydrothermally synthesized by combining Pb(NO₃)₂ and 2,6-NC₅H₃(CO₂H)₂ at 180 °C. Thermogravimetric analysis and powder X-ray diffraction measured at different temperatures indicate that Pb[NC₅H₃(CO₂)₂] displays a very high thermal stability. Photoluminescence measurement reveals that Pb[NC₅H₃(CO₂)₂] is a single component white light emitting material with a remarkably high quantum efficiency. A complete characterization including infrared and UV-vis diffuse reflectance spectroscopy, elemental analysis, and energy dispersive X-ray spectroscopy are also presented.



Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

[(L-hisH₂)MoO₂F₄]₃·H₂O and [(D-hisH₂)MoO₂F₄]₃·H₂O: Chiral molybdenum oxifluorides induced by chiral amino acids

Hongil Jo, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

In this research we used chiral amino acids, L- and D-histidine and have successfully synthesized novel chiral molybdenum oxifluorides, [(L-hisH₂)MoO₂F₄]₃·H₂O and [(D-hisH₂)MoO₂F₄]₃·H₂O (his = C₆H₉N₃O₂, histidine). Owing to the chirality of histidine, [(L-hisH₂)MoO₂F₄]₃·H₂O and [(D-hisH₂)MoO₂F₄]₃·H₂O were crystallized in chiral space group, *P*1. All the reported compounds are composed of protonated histidine and (MoO₂F₄)²⁻ ions and can be regarded as pseudo 3D structures in which all units are connected by hydrogen bonding. Circular dichroism spectra indicate that chiral compounds are enantiomers. Since the chiral compounds are noncentrosymmetric, second harmonic generation properties have been examined and they have similar efficiency to that of α -SiO₂. Other characterization such as elemental analysis, spectroscopic analysis and TGA will also be introduced in the presentation.

Poster Presentation : **INOR.P-81**

Inorganic Chemistry

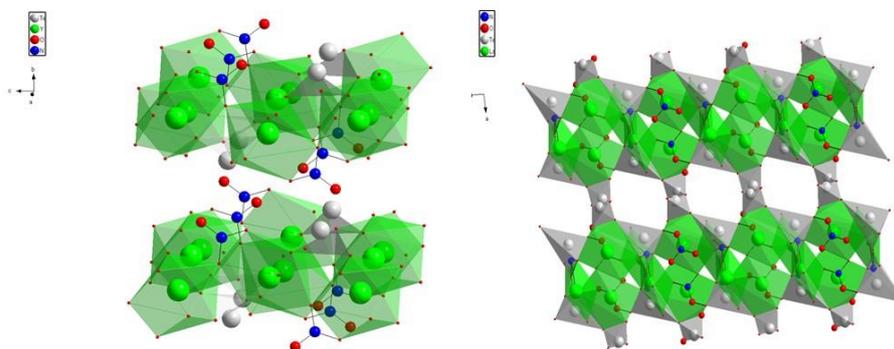
Grand Ballroom, FRI 11:00~12:30

Synthesis, structures, and characterization of two new lanthanoid tellurite nitrate compounds, $M(\text{NO}_3)(\text{TeO}_3)$ ($M = \text{Y}$ and La)

HyeEun Lee, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Two new lanthanoid tellurite nitrate compounds, $\text{Y}(\text{NO}_3)(\text{TeO}_3)$ and $\text{La}(\text{NO}_3)(\text{TeO}_3)$ were successfully synthesized. The crystal structures were determined by powder and single-crystal X-ray diffraction. $\text{Y}(\text{NO}_3)(\text{TeO}_3)$ reveals a two-dimensional (2D) layered structure that crystallizes in the orthorhombic space group, $Cmca$. $\text{La}(\text{NO}_3)(\text{TeO}_3)$, however, exhibits a three-dimensional (3D) framework structure with the monoclinic space group, $P21/c$. Both of the new compounds were fully characterized by infrared and UV–vis diffuse–reflectance spectroscopies, energy dispersive X-ray spectroscopy (EDS), and thermogravimetric analysis (TGA).



Poster Presentation : **INOR.P-82**

Inorganic Chemistry

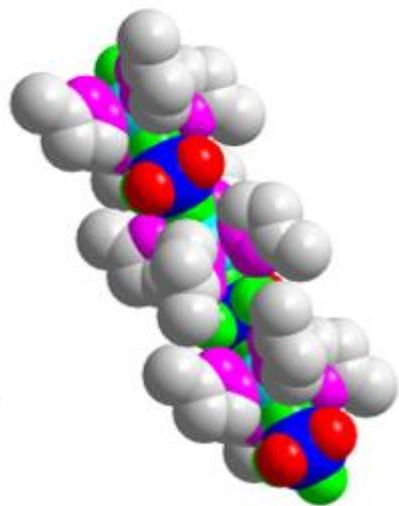
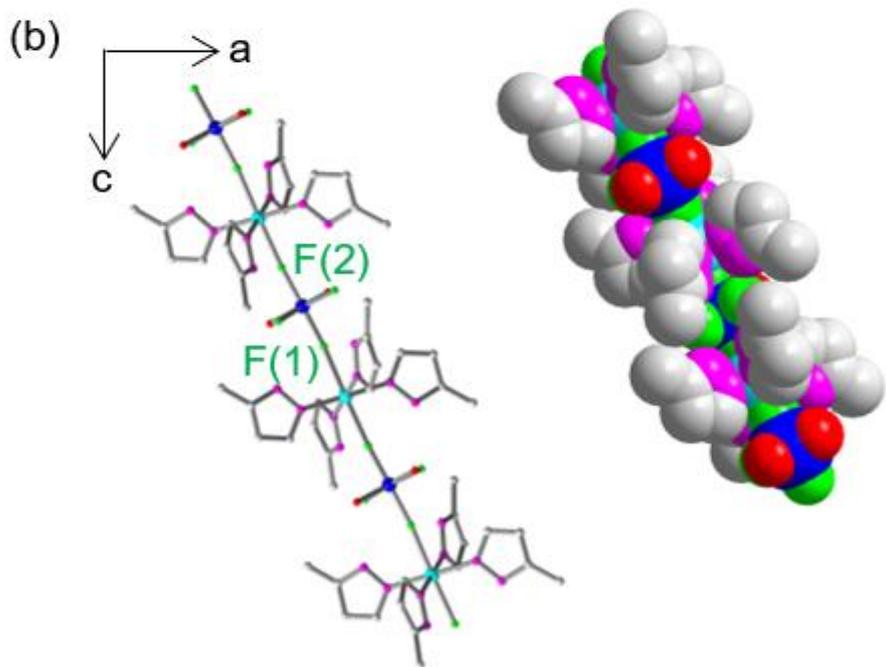
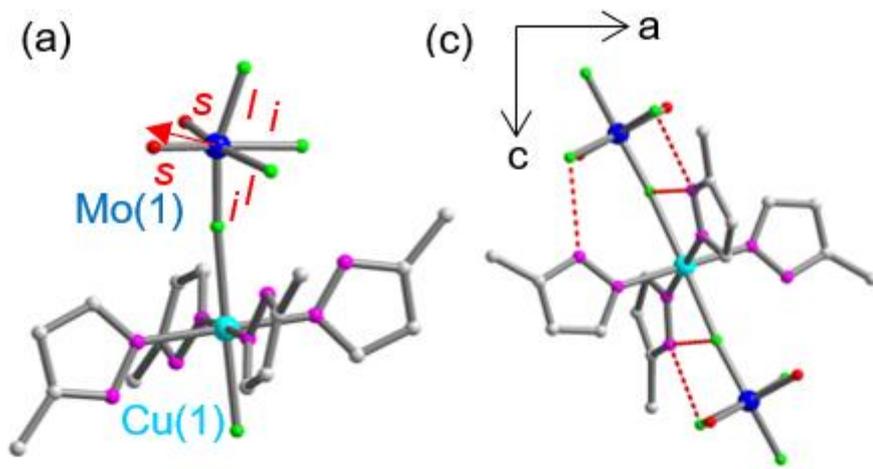
Grand Ballroom, FRI 11:00~12:30

Two New Transition Metal Oxyfluorides with Asymmetric Basic Building Units

Belal Ahmed, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Two new transition metal oxyfluorides revealing one-dimensional linear chain structures composed of asymmetric basic building units of $[\text{MO}_2\text{F}_4]^{2-}$ ($\text{M} = \text{Mo}$ and W) and $[\text{Cu}(\text{pz}/\text{mpz})_4]^{2+}$ polyhedra, i.e., $[\text{Cu}(\text{mpz})_4][\text{MO}_2\text{F}_4]$ (**1**) and $[\text{Cu}(\text{pz})_4]_2[\text{W}_2\text{F}_4]_2$ (**2**) ($\text{mpz} = 3\text{-methyl pyrazole}$; $\text{pz} = \text{pyrazole}$) have been synthesized via hydrothermal reactions. Compounds (**1**) and (**2**) crystallize in monoclinic crystal space group, $P2_1/n$ and $C2/c$, respectively. The linear chain structures are found to be attributable to the trans structure-directing anionic groups, $[\text{MO}_2\text{F}_4]^{2-}$ and hydrogen bonding interactions. Both of the title compounds show both lower-energy and higher-energy absorption band gaps, which originate from the $d-d$ transitions and the distortion of octahedral geometry of M^{2+} cations, respectively. The magnetism of $[\text{Cu}(\text{mpz})_4][\text{MO}_2\text{F}_4]$ turns out to be described by noninteracting Cu^{2+} spins rather than a spin chain due to long exchange path mediated via the nonmagnetic Mo^{6+} ions. Compounds (**1**) and (**2**) were fully characterized using spectroscopic and thermal analyses along with bond valence sum calculations.



Poster Presentation : **INOR.P-83**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Experimental and Theoretical Investigations of *n*-type Doping Effect on Thermoelectric Zintl Phase $\text{Ca}_{1.66(3)}\text{Yb}_{2.99}\text{Pr}_{0.35(1)}\text{Al}_2\text{Sb}_6$

Seong-Ji Lim, Tae-Soo You*

Department of Chemistry, Chungbuk National University, Korea

Previously, it has been reported that the *p*-type doping for thermoelectric Zintl phase $A_5M_2\text{Sb}_6$ system ($A = \text{Ca, Yb, Eu}; M = \text{Al, Ga, In}; \text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type) has successfully enhanced the maximum *ZT* values. However, *n*-type doping attempts for the system have hardly been reported. Inspired by our previously reported Zintl phase $\text{Ca}_{5-x}\text{Yb}_x\text{Al}_2\text{Sb}_6$ system, the cationic *n*-type doping was motivated for this system. Zintl phase $\text{Ca}_{1.66(3)}\text{Yb}_{2.99}\text{Pr}_{0.35(1)}\text{Al}_2\text{Sb}_6$ was synthesized by arc-melting and characterized by both powder and single-crystal X-ray diffractions. Although the targeted structural transformation through the post heat treatment which was previously proven to provoke structural transformation from the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type to the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type structure and hence increase *ZT* value, have been hard to achieve, we could confirm that the *n*-type doping to the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type phase is surely possible. According to PXRD analysis, the compound was synthesized as a single phase compound adopting the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type structure which belongs to the orthorhombic space group *Pbam* ($Z = 2$, *oP26*), with three $\text{Ca}^{2+}/\text{Yb}^{2+}/\text{Pr}^{3+}$ mixed cationic sites and four anionic sites, implying *n*-type doping was successfully applied. However, during SXRD analysis, cationic site occupations showed ambiguous site-preference. Therefore, a series of theoretical investigation for site-preference determination was performed by comparing the total electronic energies of three different model structures, where Pr atom was put into each three different cationic sites. To determine total electronic energies of each model, a series of tight-binding linear muffin-tin orbital (TB-LMTO) calculations with the atomic sphere approximation (ASA) were carried out. Consequently, energetically most favourable structure was defined, being in accordance with refined SXRD structure ' $\text{Ca}_{1.66(3)}\text{Yb}_{2.99}\text{Pr}_{0.35(1)}\text{Al}_2\text{Sb}_6$ '. Currently, attempts to achieve the structural transformation to the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type structure are underway, for *ZT* improvement.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Characteristics of 1,1-Diethyl(or 1,1-Dihexyl or 1,1-Diisopropyl)-2,5-bis{(trimethylsilyl)ethynyl}-3,4-diphenyl-silole

Jong Wook Lim, Young Tae Park^{1,*}, Ji Hun Lee

Keimyung University, Korea

¹*Department of Chemistry, Keimyung University, Korea*

2,5-Dibromo-1,1-diethyl(or dihexyl)(or diisopropyl)-3,4-diphenyl-silole as precursors can be produced by carrying out intramolecular reductive cyclization reaction of diethyl(or dihexyl)(or diisopropyl)-bis(phenylethynyl)silane treated with lithium naphthalenide, anhydrous ZnCl₂, and N-bromosuccinimide (NBS).¹⁻³ Palladium chloride, copper iodide, and triphenylphosphine as catalysts under the solvent of diisopropylamine was used to substitution react of two bromines with trimethylsilylacetylene(TMSA). The crude product was purified by recrystallization in the solvent of hexane and methanol. The product materials were characterized by ¹H, ¹³C, and ²⁹Si NMR. We also studied the electronic properties by UV-vis absorption, excitation and fluorescence emission spectroscopic methods along with electrochemical property, in particular. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2017R1D1A3B03028014).

Poster Presentation : **INOR.P-85**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Characteristics of 1,1-Diethyl(or 1,1-Dihexyl or 1,1-Diisopropyl) -2,5-bis(trimethylsilyl)-3,4-diphenyl-silole

Jong Wook Lim, Young Tae Park^{1,*}, Ji Hun Lee

Keimyung University, Korea

¹*Department of Chemistry, Keimyung University, Korea*

1,1-Diethyl(or dihexyl)(or diisopropyl)-2,5-bis(trimethylsilyl)-3,4-diphenyl-silole were manufactured by the intramolecular reductive cyclization of diethyl(or dihexyl)(or diisopropyl)bis(phenylethynyl)silane with treatment of lithium naphthalenide and followed by chlorotrimethylsilane solution in THF. After the reaction, the naphthalene was removed via using sublimation apparatus, and the crude product was purified by recrystallization. The produced materials are soluble in usual organic solvents such as THF and CHCl₃. The prepared materials were characterized by NMR, and IR spectroscopies. We also studied the electronic properties of the prepared silole derivatives by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, as well as electrochemical property such as cyclic voltametry in particular. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2017R1D1A3B03028014).

Poster Presentation : **INOR.P-86**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Ni(OH)₂ Decorated Pt Nanocubes for Electrocatalysts towards Hydrogen Evolution Reaction in an Alkaline Electrolyte

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The hydrogen evolution reaction (HER) is a critical step in many industrial processes, including water electrolysis, metal deposition, corrosion, and fuel production from CO₂ reduction. In particular, the production of H₂ through the HER in water electrolyzers has recently received large attention due to the increasing demand for H₂ gas as a key energy source for renewable energy systems. Recently, Subbaraman and co-workers demonstrated that the Ni(OH)₂ clusters electrochemically deposited on a Pt electrode could significantly enhance the HER in an alkaline medium due to a bifunctional mode. Specifically, the edges of oxophilic Ni(OH)₂ clusters promote the dissociation of water and concomitant generation of H_{ad} that subsequently adsorbs on nearby Pt surfaces and finally recombines into molecular hydrogen (H₂). This bifunctional approach presents a promising strategy for enhancing HER activity in an alkaline medium. In this work, we revealed the relationship between Pt nanocubes enclosed by {100} facets and different amounts of Ni(OH)₂ deposited on Pt {100} facets. Pt nanocubes were synthesized under CO gas atmosphere, and then Ni(OH)₂ clusters were purposely loaded on Pt surfaces. The presence of Ni(OH)₂ on Pt {100} facets was revealed by cyclic voltammetry and CO stripping experiments. Well-controlled Ni(OH)₂ clusters with different amounts on Pt nanocube surfaces showed Volcano-plot trend of HER activity in a KOH electrolyte.

Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational study of direct and asymmetric C–H activation of cyclopropanes

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Cyclopropane, which is common structural motifs of biologically active molecules have been studied in medicinal and synthetic chemistries. ¹⁻³ Applying direct C–H activation strategy, ⁴ Hong *et al.* developed asymmetric C–H activation of cyclopropane with embedding chiral directing groups to the palladium catalyst. ⁵

In this work, we have performed density functional theory (DFT) calculation to illustrate the origin of the selectivity, with analysis of the TSs of the oxidative addition step. The differences of noncovalent interactions which could stabilize the the TS were found and these distinctions suggest the rationalization for the selectivity. ⁶

Reference

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Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

The Computer-Aided Design of a Catalyst for C–H Bond Activation of Methane

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The computer-aided design of a catalyst for the methane activation is described. The putative activation of the C–H bond in methane using the Ir(III)-polypyridyl complex is investigated computationally. The computer model predicted a barrier of 35.4 kcal/mol, suggesting that the reaction should be very low-yielding, but possible at high reaction temperatures. This prediction was confirmed experimentally and subsequent analysis of the computer model revealed the key to lowering the barrier lies in increasing the softness of the Lewis basic nature of the iridium center. The computations further suggested that phosphine ligands are viable candidates and a bidentate phosphine ligand was found to give a much improved barrier of 32.3 kcal/mol. Experiments confirm that the phosphine carrying Ir-complex is an efficient catalyst for the borylation of methane. High-throughput experiments were used to optimize the reaction conditions for the catalysis and turnover numbers of ~170 were achieved at 150 • °C.

Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

New 2D Porphyrinic Metal-Organic Frameworks: Synthesis and Property

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As the number of MOFs increases, it is important to create an optimal structure for various applications. The attractive advantage of MOFs is that the structure can be “designed” with a variety of components to suit its purpose. Especially, topological analysis of designed framework helps to fine structural property by selecting metal clusters and organic ligands. Recently, flexible MOFs have been studied by many research groups. The flexible MOFs react to external stimuli, such as removal/uptake of guest molecules, temperature, and pressure¹⁻². Physical and mechanical stimuli cause transformation of the framework. In this work, we synthesized transformable 2D MOFs, PPF-300 and PPF-301 (PPF = Porphyrin Paddlewheel Framework), constructed from Zn paddlewheel SBUs and flexible porphyrin ligands. Interestingly, topological analysis shows flexibility and relationship of two structure.

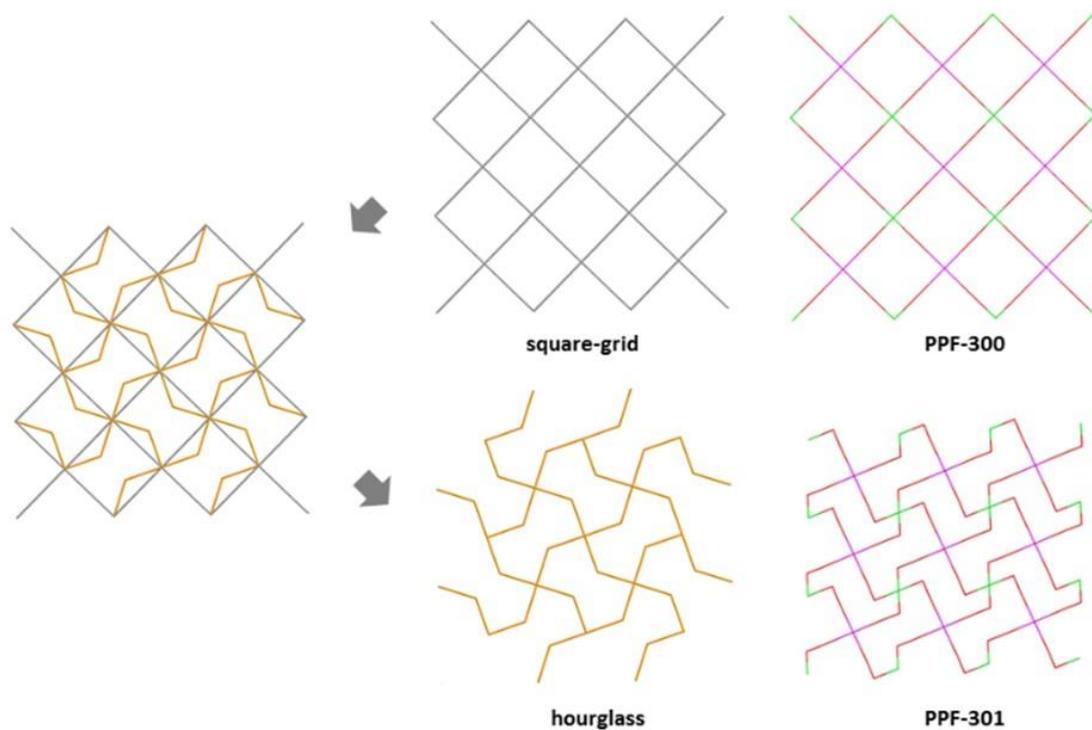


Figure 1. Schematic representation of relation between square-grid of PPF-300 and hourglass of PPF-301 tessellation. The square-grid has a close relation to hourglass as conformation of flexible fragment.

Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Supramolecular Pt(II) and Ru(II) Trigonal Prismatic Cages Based on a Tris(pyridyl)borane Donor

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The boron-containing π -conjugated compound, tris(2,6-dimethyl-4-(2-(pyridin-4-yl)ethynyl)phenyl)borane, was synthesized as a new electron donor system with Lewis acidic properties in supramolecules. Self-assembly of tripyridyl borane ligand and diruthenium or platinum electron acceptors erected trigonal prismatic ruthenium-boron (Ru-B) and platinum-boron (Pt-B) cages. These complexes were characterized by various analytical techniques including ¹H, ¹¹B, diffusion-ordered NMR spectroscopy (DOSY), electrospray ionization mass spectrometry (ESI-TOF-MS), and X-ray crystallography. The solid-state structure of supramolecular Ru-B cage was ascertained to its molecular connectivity between electron donors and electron acceptors with an inner space of about 400 Å³. The binding properties of complexes with fluoride through the empty p-orbital of tris(pyridyl)borane donor and Pt-B cage were studied in acetone solution. Upon the complexation of borane ligand and Pt-B cage with a fluoride ion, significant changes were observed in ¹H and ¹¹B NMR spectra because the geometries of boron centers altered from trigonal planar coordination to tetrahedral one. Furthermore, in UV-visible absorption spectra, the maximum absorption of tris(pyridyl)borane ligand at 357 nm was dwindled upon the addition of incremental amounts of fluoride and new band around 340 nm was assignable to π -p π (B) charge transfer (CT) transition of the triarylborane-center. The fluoride binding constant of tris(pyridyl)borane ligand was estimated as $2.0 \times 10^6 \text{ M}^{-1}$ in acetone from the 1:1 binding isotherm. In case of Pt-B cage, it exhibited a strong low-energy absorption at 365 nm that was gradually quenched upon addition of fluoride anions. When the excess fluoride was present in a solution of Pt-B cage, a red shift was observed in the absorption spectra due to the lowering of the LUMO level by the coordination of pyridyl lone pair electrons to the Pt core. The binding constant of Pt-B cage with the fluoride ion was estimated as $1.3 \times 10^{10} \text{ M}^{-2}$ in acetone based on the 1:2 binding isotherm, whereas Ru-B cage was found to be unstable in the existence of fluoride ions.

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Tetra-, Hexa-, Dodeca-Nuclear Ir(III) Supramolecules via Bridge-Driven Self-Assembly

Seul Gi Lee, Ji Yeon Ryu, Junseong Lee*

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The bridge-driven self-assembly provides a new simple strategy and can be used in the various homo- or hetero-metallic three-dimensional self-assemblies. Previously, we reported the half-sandwich ruthenium complexes using tetrazolyl ligands, in which two interesting binding mode (μ_2 -bridging and η^2 -chelating) of tetrazolyl ligand toward two metal centers was observed. It is worthy to note that μ_2 -bridging mode of tetrazolyl ligands have not been used in the self-assembly of supramolecular cages. Therefore, we adapted the μ_2 -bridging mode of tetrazolyl groups which bind two half sandwich iridium(Ir) (III) complexes to construct concrete supramolecular architectures. It provides strong bonds toward Ir metal centers. In addition, due to the diversity of bridging mode of tetrazolyl group, the structures of Ir(III) supramolecules could be modulated by changing the numbers and the position of tetrazolyl units of ligands. From 1,2-, 1,3-ditetrazolyl benzene and 1,3,5-tritetrazolyl benzene, three new Ir(III) supramolecules were synthesized via bridge-driven self-assembly and characterized by IR, ^1H , ^{13}C NMR spectroscopy, and Electrospray ionization mass spectrometry. Additionally, their structures were determined by single crystal X-ray crystallography. The bridging modes of tetrazolyl ligands influence to the architectures of Ir supramolecules such as rectangular, truncated trigonal pyramidal and truncated tetrahedral structure. The rectangular structure was obtained from the reaction of 1,2-ditetrazolyl benzene, $[\text{Cp}^*\text{IrCl}_2]_2$, AgOTf in molar ratio of 1:1:3. By changing the positions of tetrazolyl groups 1,2-ditetrazolyl benzene to 1,3-one, truncated trigonal pyramidal hexa-iridium supramolecule was obtained. Even more interesting truncated tetrahedral structure was achieved by the reaction of 1,3,5-tritetrazolyl benzene, $[\text{Cp}^*\text{IrCl}_2]_2$, AgOTf in molar ratio of 2:3:9.

Poster Presentation : **INOR.P-92**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

New Type of Titanium Complexes with Chiral Tridentate Ligand for Cycloaddition of CO₂ to Epoxide

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CO₂ as C1 block had led to a great deal of attention environmentally and economically. In particular, the copolymerization reaction with epoxide, one of the most efficient methods of CO₂ utilization, has been regarded as an interesting and challenging task for many researchers. Utilization of CO₂ to epoxide copolymerization produces high value-added materials such as polycarbonates (PCs) and cyclic carbonates (CCs). Although lots of complexes have already been developed successfully as catalytic system to produce polycarbonates (PCs) from the copolymerization of CO₂ and epoxide, catalytic system for cyclic carbonates (CCs) is not well developed yet and searching for the efficient catalysis is still remained as an important research area. We synthesized a series of new titanium complexes, TiLCl₂(THF)(**1**) and TiL₂(**2**), containing tridentate chiral [ONO] type Schiff-base ligand, **L**, easily prepared from the condensation reaction of 2,4-pentadione and (1R,2S)-(-)-1-aminoindanol. Synthesized Ti complexes were characterized by various analytical methods including X-ray crystallography. Ligand **L** acted as a dianionic tridentate ligand and, owing a chiral center in the aminoindanol part, imparted chirality to its titanium complexes. Complexes **1**, **2** and previously reported analogues Ti complexes(**3-5**) were used as catalysts in the cycloaddition of CO₂ to propylene oxide as the first representatives of titanium complexes with tridentate schiff-base ligand to have been used for this purpose. These complexes provided high selectivity toward cyclic propylene carbonate (>99%) and showed considerable activities with TOF values up to 131 h⁻¹ in comparison with the previously reported catalyst systems.

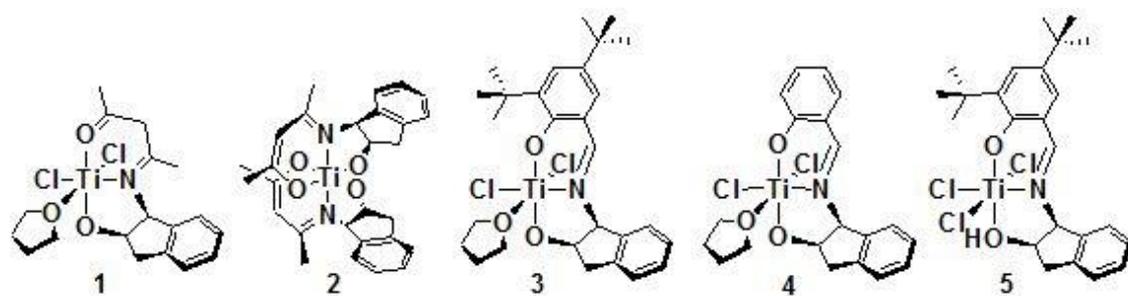


Figure 1. Molecular structures of Ti complexes with chiral tridentate ligands (1-5).

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cycloaddition of Carbon Dioxide to Cyclic Carbonate with Cobalt(III) Catalytic System Containing Tetradentate [ONNO] Type Ligand Derived from Pyridoxal

Sam Hwang, Ji Yeon Ryu, Junseong Lee*

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As a result of global warming, reduction of carbon dioxide is a major interest in industry. One of the efficient methods using CO₂ as an industrial material is the synthesis of cyclic- or poly- carbonate through ring opening reaction of propylene oxide with homogeneous catalyst. Co complexes containing SALEN(N,N'-bis(salicylidene)ethylenediamine) ligand have been reported as a successful catalytic system in the reaction. In this study, the new cobalt complex containing SALEN ligand with pyridine was synthesized for developing new Co(III) system used in transformation of carbon dioxide. We expected that cationic moieties in ligand can replace co-catalysts. A new cobalt(III) complex of pyridoxyl SALEN ligand was synthesized by the reaction of pyr2en ligands (pyr2en = (N,N'-bis(pyridoxylideneiminato)ethylene)) with Co(OAc)₂. The complex was characterized by various analytic methods such as infrared spectroscopy, high resolution mass analysis, and single crystal X-ray crystallography. The tetradentate Schiff base ligand binds cobalt metal in a plane and forms an octahedral geometry by coordinating acetate and DMSO. The synthesized cobalt complex was used in the cycloaddition reaction of CO₂ to propylene oxide and the detailed study will be presented.

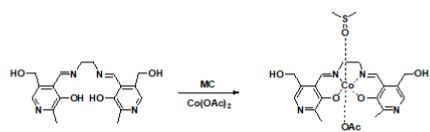


Figure 1: Synthesis of Co(III) complex

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of water-soluble Ruthenium Nitrosyl Complexes with Schiff base ligand

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Nitric oxide plays important roles in a wide variety of physiological processes, including neurotransmission, immune response, blood pressure control, and inhibition of tumor growth. For the purpose of controlling the physiological processes, compounds that selectively release nitric oxide have attracted considerable interest. Among them, ruthenium nitrosyl complexes have been proposed as a photodynamic therapeutic agents in biomedicine and in tumor treatment. Previously, we researched ruthenium nitrosyl complex with salophen ligand, $[\text{Ru}(\text{III})(\text{NO})(\text{salophen})\text{Cl}]$. This research aims at developing ruthenium nitrosyl complexes which absorb long wavelength visible light to release NO and are dissolved in water. We introduced new ligands with hydroxyl group on the positions of ortho, meta and para of the salophen ligand in order to increase the solubility in water. In this study, we show the NO-releasing properties of the complexes monitored by UV-VIS, IR spectroscopy and EPR.

Poster Presentation : **INOR.P-95**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Elucidating a Supramolecular Catalyst for C–H Activation through Electronic Structure Calculations

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One of the major challenges in chemistry is to understand how Nature handles biochemical processes very efficiently using metalloenzymes. To understand the structure-function relationship of metalloenzymes, many catalysts are synthesized to mimic the enzymes. Alternatively, supramolecular hosts can mimic the enzymes due to the unique shapes provided by them. One of the recent popular host molecules is cucurbituril (CB), a pumpkin shaped molecule. Based on the number of monomer units, the host can accommodate guests of different sizes. Due to the presence of hydrophilic portals and a hydrophobic core, this host can accommodate a range of molecules such as cations (more preferable), anions (cation assisted) and even neutral gases molecules. Vanadium (IV) oxo species (V=O) are known to be found in the active site of the vanadium-dependent halo-peroxidase enzyme. This enzyme catalyzes the two electron oxidation of a halide (X⁻) by hydrogen peroxide (H₂O₂) to form the corresponding hypohalous acid (HOX). Recently, a V=O species bound to CB-[6] was reported which oxidizes n-pentane to 2-pentanol. The catalyst is very selective which oxidizes only n-pentane but not cyclo-octane or styrene. Unfortunately, the catalyst structure or the possible reaction mechanism for the selectivity is unknown. We have proposed the possible geometric structure of the catalyst through electron structure calculations. A possible reaction mechanism for C–H activation is proposed. References 1. Lee, J. W.; Samal, S.; Selvapalam, N.; Kim, H.-J.; Kim, K. *Acc. Chem. Res.* 2003, 36, 621–630. 2. de Lima, S. M.; Gomez, J. A.; Barros, V. P.; Vertuan, G. S.; Assis, M. D.; Graeff, C. F. O.; Demets, G. G. J.-F. *Polyhedron*, 2010, 29, 3008–3013.

Poster Presentation : **INOR.P-96**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Deposition Method of High-purity Titanium Dioxide Crystalline Nanoparticle Having Core/Shell Structure and Its Application

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Abstract Crystalline titanium dioxide nanoparticles(nano-TiO₂) is being applied to biosensors, next generation secondary battery electrodes, solar cells, and nanoelectronic devices, which are key materials for next generation. In this work, Nanocrystalline titanium dioxide particles (nano-TiO₂) were directly synthesized using decomposition of gas-phase titanium tetrachloride (TiCl₄) by microwave plasma torch. In order to improve the semiconductor characteristics of TiO₂, the ratio of amounts for the two crystal structures (anatase and rutile) of titanium dioxide was controlled by adjusting the flow rates of injection of oxygen and hydrogen into the plasma-torch, and the synthesized titanium dioxide was deposited on a silicon wafer. Their crystal structures were evaluated using X-ray diffractometer(XRD). The nanoparticle size and growth rate of the nano-TiO₂ was controlled by the microwave power, the argon gas and the oxygen gas flow rate, and evaluated by scanning electron microscope (SEM) and dynamic light scattering system(DLS). A suitable solvent treatment was applied to increase the adsorption power of nano-TiO₂ and silicon wafers. And the nano-TiO₂ can be realized as a core/shell structure through atomic layer deposition(ALD) process and confirmed by transmission electron microscope(TEM). The synthesized core/shell nanoparticles were evaluated for their electrical properties by applying the photoelectrode of a dye-sensitized solar cell (DSSC).

Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaluation of particle size change and polyol purification ability of magnesium silicate according to synthesis conditions.

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The magnesium silicate, which is a porous material, purifies the polyol contained impurities using adsorption. After purification of the polyol through adsorption, the magnesium silicate is separated through a filtration process. Filtration time and purification capacity are inversely related to each other, and these interactions are closely related to the particle size of its. The magnesium silicate manufactured by the reaction of water glass solution and magnesium sulfate was synthesized by changing the reaction conditions such as temperature, injection rate and mole ratio of reactants and analyzed the particle size and Si/Mg composition ratio according to the reaction conditions. The magnesium silicate was prepared as a purification powder through drying and grinding process and the polyol purification ability of magnesium silicate according to each reaction condition was compared and evaluated. The mole ratio of Si/Mg and the concentration of starting materials in the reaction conditions had the greatest effect on particle size and purification ability. The higher the mole ratio of Si/Mg and the higher the starting material concentration, the better the purification ability. As a result of the evaluation of the average particle size according to the reaction conditions, the average particle size had no significant effect on the filtration time and the small nanoparticles of below 1 μm after the grinding process had a great influence the filtration time. As the amount of the generated nanoparticles increases, the purification ability is better. However, the filtration time is prolonged due to the clogging of the filter paper with the nanoparticles, resulting in a decrease in the productivity by reason of the delay in the synthesis time and the purification time.

Poster Presentation : **INOR.P-98**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaluation of polyol purification ability and characterization of magnesium silicate dependent on magnesium source

Jhong Ryul Yoo, Sungho Park^{1,*}

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¹*Department of Chemistry, Daejin University, Korea*

The magnesium silicate, which is a porous material, purifies the polyol contained impurities using adsorption. After purification of the polyol through adsorption, the magnesium silicate is separated through a filtration process. Filtration time and purification capacity are inversely related to each other, and these interactions are closely related to the particle size of its. The magnesium silicate manufactured by reacting magnesium solution with water solution was synthesized by changing reaction conditions such as magnesium source (MgCl₂, MgSO₄, Mg(NO₃)₂) and mole ratio of reactants and analyzed the changes of particle size and Physical property, and Si/Mg composition ratio according to reaction conditions. The synthesized magnesium silicate is prepared as a powder for purification through a drying and grinding process. After the purification, the pH of the polyol and the filtration time were measured to compare the purification ability. The Si/Mg composition ratio of the magnesium silicate was measured as 3.8~4.8, and the Si contents were increased in the order of MgCl₂, MgSO₄, Mg(NO₃)₂. The physical strength at the grinding process increased with increasing Si/Mg composition ratio of magnesium silicate. That is, the higher the Si content is, the more the strength of the silicate is increased. Also, the Si content was more influenced by the magnesium source than by the reactant molar ratio of water glass. As the physical strength increased, the average particle size increased from 17 μm to 30 μm and the number of nanoparticles below 1 μm decreased. Therefore, as the physical strength of the magnesium silicate increased, the amount of nanoparticles clogging the filter paper was reduced, thereby improving the productivity by shortening the purification filtration time.

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Investigation of Terphenyl Benzimidazole Isomer effect for the efficient electron transporting layer in blue PHOLED

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Recently, various types of electron transport material (ETM) are reported and high triplet energy ETMs for blue PHOLED are also reported by various research groups. For the highly efficient blue PHOLED, high triplet band gap ETM is required to confine the triplet light emission in emission layer in OLED. At the same time, high electron mobility is also needed. However, to design and synthesis of the high triplet energy with high electron mobility material is challengeable due to the tradeoff relationship between triplet energy and electron mobility. In this research, we have designed and synthesized three different terphenyl backbone (ortho-, meta-, and para-terphenyl) based benzimidazole ETMs to understand structure-properties relationship and we are aiming to suggest the design strategy of the high triplet energy with high electron mobility ETM. The photophysical and electrochemical properties of the three different benzimidazole terphenyl isomers were compared each other. In the photophysical and electrochemical properties, the ortho and para isomers show charge delocalization properties through imidazole and terphenyl moiety in the different pathway, which showing the through space (ortho) and through bond (para) delocalization. Due to the efficient charge delocalization by the through bond pathway, the para isomer results low triplet energy gap, which is not suitable for blue PHOLED. In contrast, meta isomer shows charge localization property and results high triplet energy gap. In the DFT/TDDFT calculations, this result is well agreed with experimental data. In conclusion, the ortho isomer is suitable for the high triplet energy with high electron mobility properties due to the through space charge delocalization by the through space pathway.

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Emission Color Tuning from Non-conjugated Backbone based Donor-Acceptor Molecule Induced Thermally Activated Delayed Fluorescence and their TSCT Effect Control

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Thermally activated delayed fluorescence (TADF) molecules have evolved rapidly as the new-generation materials for application in organic light diodes (OLEDs). We synthesis a novel molecular design for thermally activated delayed fluorescence (TADF) molecules based on a non-conjugated Xanthene backbone(2,7-di-tert-butyl-9,9-dimethyl-xanthene) with through-space charge transfer (TSCT) effect between each Electron Donor(D) and Electron Acceptor(A) functional groups. We examined 6 different diphenyl amine donors (OMe, t-Bu, CH₃, H, F, CN) with different electron donating characters to control the photo-luminescence. These molecules are identified by through-space charge transfer for emitting fluorescence. The non-conjugated molecules avoid the direct charge transfer effect, induce of through-space charge transfer. The structures position of the donor and acceptor with co-facial alignment at distances of about 7.5-8.5 Å wherein efficient spatial charge transfer can occur. To control the color of the emission, change the electron donor property to systematic and measure photophysical and electrochemical properties. To identify the structural and electronic properties of molecules, DFT and TD-DFT calculations were used to compare the experimental properties. The results showed that these molecules had effective TADF and were able to tune by blue to green colors in DCM solvent.

References

- [1] Wee, K.-R. et al. J. Org. Chem. A . 2009, 74, 8472-8475
- [2] Tsujimoto, H. et al. J. Am. Chem. Soc. 2017, 139, 4894-4900
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Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

All-in-One Derivatized Tandem p⁺n-Silicon-SnO₂/TiO₂-Dye Molecules Water Splitting Photoelectrochemical Cell

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Mesoporous metal oxide film electrodes consisting of derivatized 5.5 μm thick SnO₂ films with an outer 4.3 nm shell of TiO₂ added by atomic layer deposition (ALD) have been investigated to explore unbiased water splitting on p, n, and p⁺n type silicon substrates. Modified electrodes were derivatized by addition of the water oxidation catalyst, [Ru(bda)(4-O(CH₂)₃PO₃H₂)-pyr]₂, 1, (pyr = pyridine; bda = 2,2'-bipyridine-6,6'-dicarboxylate), and chromophore, [Ru(4,4'-PO₃H₂-bpy)(bpy)₂]²⁺, RuP²⁺, (bpy = 2,2'-bipyridine), which form 2:1 RuP²⁺/1 assemblies on the surface. The SnO₂/TiO₂-chromophore-catalyst assembly was integrated with the Si electrodes by a thin layer of titanium followed by an amorphous TiO₂ (Ti/a-TiO₂) coating as an interconnect. In the integrated electrode, p⁺n-Si-Ti/a-TiO₂-SnO₂/TiO₂-2RuP²⁺/1, the p⁺n-Si junction provided about 350 mV in added potential to the half-cell. At pH 5.7 in 0.1 M acetate buffer, these electrodes with a fluorine-doped tin oxide (FTO) back contact under ~1 sun illumination (100 mW/cm²; white light source) perform efficient water oxidation with a photocurrent of 1.5 mA/cm² with an 88% Faradaic efficiency (FE) for O₂ production at an applied bias of 600 mV versus RHE. In photolysis experiments at pH 5.7 in 0.1 M acetate buffer, bias-free photocurrents approaching 100 μA/cm² were obtained for water splitting, 2H₂O → 2H₂ + O₂. The FE for water oxidation was 79% with a hydrogen efficiency of ~100% at the Pt cathode.

Poster Presentation : **INOR.P-102**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Controlling the Electronic Structure of 1,6-Triphenylamine Substituted Pyrene for Wide-Range Emission Color Tuning

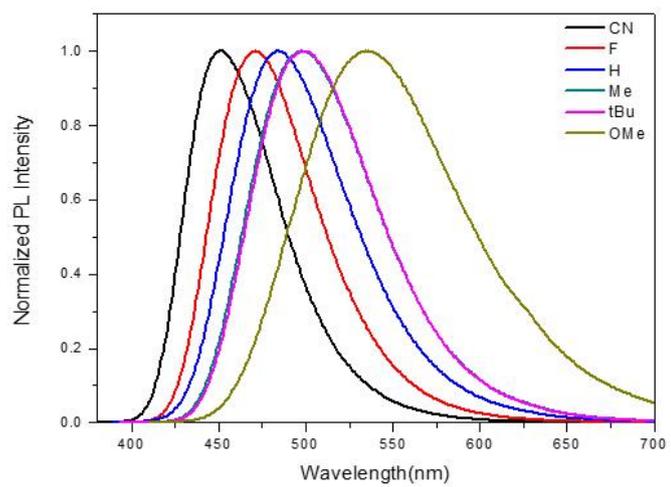
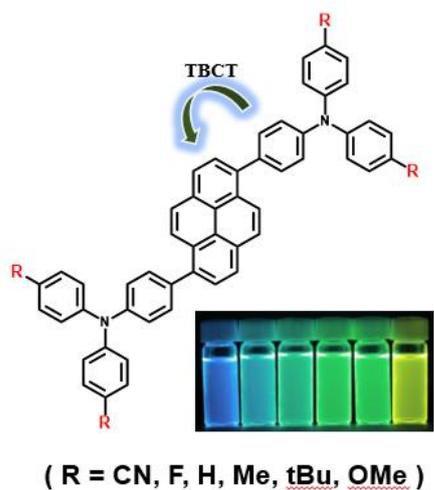
Kyeong Min Lee, Kyung-Ryang Wee*

Department of Applied Chemistry, Daegu University, Korea

Pyrene is possible to connect electron withdrawing, donating groups at suitable position, which can result in enhanced intramolecular charge transfer. Herein, a facile strategy to tune the emission color has been established to the triphenylamino donor at the 1,6-position on the pyrene-based chromophores by Suzuki coupling reaction. We demonstrated differing distinctive emission properties both in solution and in the solid state simply by fine-tuning of the 1,6-position substitutions of the pyrene core. Broad and tunable emission, from blue to orange wavelengths, were observed in dilute solutions. We can explained intramolecular charge transfer from donor to acceptor by solvatochromism and Lippert-Mataga plot. Also, Photophysical properties could be explained by UV, CV, PL, film PL, life time, quantum yield and by the density functional theory calculations.

Reference

- (1) Wee, K.-R. et al. *J.Org.Chem.*2009, 74, 8472–8475.
- (2) C.-Z. Wang et al. *J. Org. Chem.*, 2017, 82, 7176–7182



Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Perylene-Based Emission Color Tuning – Dependent on electron - donating and -withdrawing nature of the diarylamine substituents

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A series of perylene-based emitters, 3,9-Bis(*p*-(R)-diphenylamino)perylene, were synthesized by Buchwald-Hartwig cross-coupling reaction of 3,9-dibromoperylene with *p*-(R)-diphenylamine. An approach to control the emission color of the perylene-based emitting materials is demonstrated. Following the strategy, by introducing variety of diarylamine derivatives with electron donating or electron withdrawing R groups, emission colors were efficiently controlled from green to red. On the basis of solvatochromic experiments, these chromophores showed through-bond intramolecular charge transfer character in order to increasing the solvent polarity. In particular, depending on the electron push-pull substitution the different charge transfer character was showed which showing lower charge transfer property in the electron withdrawing substitution. Detailed photophysical and electrochemical studies on a series of perylene were also investigated as well as DFT/TDDFT calculations.

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Copper(II) Complexes Containing *N'*-Substituted *N,N'*,*N*-Bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)amine Derivatives: Synthesis, Characterization and Application Towards Rac-lactide Polymerization.

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We have synthesized new series of Cu(II) complexes with ligands L_n ($L_n = L_A - L_F$) ($L_A = N,N$ -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine, $L_B = 4$ -methoxy- N,N -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine, $L_C = 4$ -fluoro- N,N -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine, $L_D = 2,4,6$ -trimethyl- N,N -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine, $L_E = 2,6$ -diethyl- N,N -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine, $L_F = 4$ -isopropyl- N,N -bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine). All complexes were characterized by various spectroscopic methods. The catalytic properties of these complexes toward the polymerization of rac-lactide (LA) in the presence of MeLi were investigated at -25 °C and room temperature.

Poster Presentation : **INOR.P-105**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Characterizations of Copper(II) Complexes Containing Tridentate *N,N',X*-Iminomethylpyridines

Jaegyeong Lee, Hyosun Lee*

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We have synthesized and characterized a series of new copper(II) complexes, namely [**L_nCuCl₂**] supported by ligands L_n (L_n = L_A – L_F) (L_A = (*E*)-*N*¹,*N*¹-dimethyl-*N*²-(pyridin-2-ylmethylene)ethane-1,2-diamine, L_B = (*E*)-2-methoxy-*N*-(pyridin-2-ylmethylene)ethanamine, L_C = (*E*)-2-(piperidin-1-yl)-*N*-(pyridin-2-ylmethylene)ethanamine, L_D = (*E*)-2-morpholino-*N*-(pyridin-2-ylmethylene)ethanamine, L_E = (*E*)-*N*¹,*N*¹-dimethyl-*N*³-(pyridin-2-ylmethylene)propane-1,3-diamine and L_F = (*E*)-3-methoxy-*N*-(pyridin-2-ylmethylene)propan-1-amine). New copper(II) complexes are characterized by spectroscopic methods such as ¹H-NMR, IR, elemental analysis and X-ray crystallography. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) were investigated at 60 °C.

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Characterization of Zinc(II), Cobalt(II) and Cadmium(II) Complexes Containing 4-Isopropyl-*N,N*-bis((1H-pyrazol-1-yl)methyl)benzenamine Derivatives

Solhye Choe, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of Zn(II), Co(II) and Cd(II) complexes with ligands **L_A** and **L_B** where **L_A** is 4-isopropyl-*N,N*-bis((1H-pyrazol-1-yl)methyl)benzenamine and **L_B** is 4-isopropyl-*N,N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine. All complexes were characterized by various spectroscopic methods. The polymerization of methyl methacrylate (MMA) in the presence of MMAO by of all complexes was investigated at 60 °C.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Folate conjugated hollow microporous organic networks for targeted drug delivery

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Due to their porosity, high surface areas, and chemical stability, the microporous organic networks (MONs) have a great potential as drug delivery materials. This presentation shows that hollow and microporous organic network spheres decorated with folic acids (H-MON-FA) were prepared using silica templates by the Sonogashira coupling of organic building blocks and successive post-synthetic modification. The drug (DOX) delivery performance of H-MON-FA to cancer cells was studied. When we treated the cancer cells with DOX/H-MON-FA, the cell viabilities decreased to 62, 49, 43, 41, 38, and 33% with DOX quantities of 0.1, 0.25, 0.5, 1, 2.5, and 5 $\mu\text{g/mL}$, respectively after 24 hours. After 48 hours, the cell viabilities further decreased to 45, 35, 33, 31, 28, and 18% with DOX quantities of 0.1, 0.25, 0.5, 1, 2.5, and 5 $\mu\text{g/mL}$, respectively. In comparison, when we treated the cancer cells with DOX/H-MON, the cell viabilities decreased to 80, 70, 57, 55, 54, and 50% with DOX quantities of 0.1, 0.25, 0.5, 1, 2.5, and 5 $\mu\text{g/mL}$, respectively after 24 hours. After 48 hours, the cell viabilities further decreased to 67, 52, 44, 42, 40, and 33% with DOX quantities of 0.1, 0.25, 0.5, 1, 2.5, and 5 $\mu\text{g/mL}$, respectively. These results imply that H-MON materials have a promising potential as a drug carrier due to their high porosity. Also, the possibility of tailored surface modification of H-MON materials is beneficial to develop the drug delivery materials.

Poster Presentation : **INOR.P-108**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cu(I) Coordination Polymer Based on Thionated Pyromellitic Diimide

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Department of Chemistry, Gyeongsang National University, Korea

In the previous studies, four copper(I) coordination polymers were prepared by reaction of CuI and *N,N'*-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide (**L_o**) under varying solvent conditions. The coordination polymers exhibited reversible solvent exchange and crystal transformation by exposure to vapors of volatile organic compounds. In this study, we tried to introduce soft S atoms instead of carbonyl oxygen atoms to the pyromellitic diimide (**L_o**). *N,N'*-bis[2-(cyclohexylthio)ethyl]pyromellitic dithioimide (**L_s**) was prepared by thionation of *N,N'*-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide with Lawesson's reagent. A Cu(I) coordination polymer (CP) was prepared by the reaction of CuI and **L_s**. Structural characterization, thermal and photoluminescent properties of new Cu(I) coordination polymer are presented.

Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Crystal Structures of Copper(I) Coordination Polymers Based on 6-(2-(benzylthio)ethyl)-5H-pyrrolo[3,4-b]pyridine-5,7(6H)- dione

Mun JunHa, Hansu Im, Juhyeon Park, Tae Ho Kim*, Jineun Kim*

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6-(2-(benzylthio)ethyl)-5H-pyrrolo[3,4-b]pyridine-5,7(6H)-dione (**L**) was synthesized by the reaction of pyridine dicarboxylic anhydride and 2-(benzylthio)ethylamine. Yellow ligand crystals were grown by slow evaporation in a MeOH/DCM mixed solvent. Red copper(I) coordination polymer $\{[\text{Cu}_3\text{I}_3\text{L}]\}_n$ (CP) was obtained by the reaction of CuI and **L** at a ratio of 3: 1, crystallized in space group monoclinic $P2_1/c$. The asymmetric unit is composed of three CuI and an **L**. In the crystal, Cu_3I_3 units were infinitely linked along the a-axis. The $\{\text{Cu}_3\text{I}_3\}_n$ chains along [020] and [002] directions are linked by **Ls** and the $\{\text{Cu}_3\text{I}_3\}_n$ chains along [020] and [002] directions are also linked by another **Ls**. Therefore, CP forms a three dimensional frame work. All copper atoms have distorted tetrahedral coordination environments. Cu1 is coordinated by one nitrogen, one sulfur and two iodine atoms, and Cu2 and Cu3 are coordinated by four iodine atoms. UV, IR and TGA were used to characterize physicochemical properties and thermal stability of CP.

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Real-Time Colorimetric Detection of Water in Organic Solvents by Dipolar Dye Incorporated into AlPO₄-5 Nanochannel

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Trace water could serious influences not only the yield of production of chemicals but also their activity and application. Accurate and rapid quantitative detection of trace water in gases or liquid organic products is of great importance in chemical industrial processes, environmental monitoring for maintaining the quality, yield, or reliability of the final product. The dipolar dye with dimethyl amine confined inside AlPO₄-5 matrices have recently emerged as a novel type of functional optical materials. Recently, a simple and low-cost optical reflectance sensor materials has been developed based on the dipolar dyes confined inside AlPO₄-5. This AlPO₄-5/dye composites was successfully employed in a optical type humidity sensing material with high responsivity. For instance, the dipolar dye with dimethyl amine confined inside AlPO₄-5 exhibits excellent properties as humidity sensor in terms of sensitivity (much lower than 200 ppm), response time (around 10 second). We demonstrate that the humidity sensitivity stems from Brønsted-Lowry acid site in AlPO₄-5 channels. When water molecules enter into AlPO₄-5 channels, the dimethyl amine in dipolar dye is protonated by Brønsted-Lowry acid site in AlPO₄-5, framework, which causes the color to change due to reducing donor- acceptor intra-charge transfer in the dipolar dye. Also the benefits of the dye encapsulation inside the AlPO₄-5 channels in terms of stability at various temperature have also been presented.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and characterization of Cu(II) complexes bearing 2-thienylmethyl and 2-naphthalenylmethyl derivate of (R,R)-1,2-diaminocyclohexane and its application toward asymmetric Henry reaction

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Homo-chiral Cu(II) complexes with N-(2-thienylmethyl)-N'-(2-naphthalenylmethyl) -(R,R)-1,2-diaminocyclohexane (TNDC) ligand was synthesized and characterized. The X-ray crystal structure of Cu(II) complex containing TNDC was determined. The geometry around the Cu(II) centre for (TNDC)CuCl₂ was distorted square-planar. Catalytic activities of (TNDC)CuCl₂ and (TNDC)Cu(OAc)₂ with 10 mol% of diisopropylethylamine in the asymmetric Henry reaction of aldehyde(benz-, 3-phenylpropion-, isovaler-, n-butyl-) and nitro-methane was examined.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Exfoliated graphite electrodes for organic single crystal field effect transistor Devices

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Organic single crystals are ideal platform for deeper understanding the inherent electrical characteristics of organic molecules thanks to its feasibility in fabrication into conventional electronic devices, such as field effect transistor (FET). When a target organic crystal is fabricated into an electronic device, an important component that requires a careful attention is the electrode, which is in direct contact with the material, and is generally used by depositing metals. However, the metal electrode may damage the organic crystal in the process of deposition, and it is expensive and ineffective especially for organic crystals having various sizes and morphologies. Thus, it is important to develop a new contact electrode system for organic crystal devices. we present here a method for implementing an organic single crystal field effect transistor using exfoliated graphite as contact electrodes. Compared to the case of using conventional metal as the electrode, we confirmed the similar or improved the performance of the devices with respect to charge carrier mobility and contact resistance. Furthermore, by increasing the concentration of -OH groups on the surface of the graphite electrodes by oxygen plasma treatment, the work function of graphite could be modulated to a certain degree. Through this treatment, it was possible to minimize the injection barrier at the contact between the graphite electrodes and target organic crystal by matching the work function of graphite with the HOMO level of the picene single crystal. Through this study, it was confirmed that exfoliated graphite could be applied as an electrode material in the organic molecular crystal devices.

Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Titanium-Carboxylate Metal-Organic Framework Bases on an Unprecedented Ti-oxo Chain Cluster

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Development of new titanium-based metal-organic frameworks (MOFs) with high crystallinity has been attracting significant research attention because it allows understanding of the structure-property relationship in their photocatalytic applications. Herein, we present a new single crystalline titanium-carboxylate MOF (1), which is built up from a porphyrinic linker and the unprecedented Ti-oxo chain cluster. 1 exhibits high porosity, large surface area, and also strong absorption in the visible light region. The photocatalytic activity of 1 was investigated by detecting generated singlet oxygen (¹O₂), superoxide (O₂⁻), in addition to the selective oxidation of benzyl alcohol to benzaldehyde upon the visible light (400-800 nm) irradiation

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Vertically aligned growth of single crystal titanyl phthalocyanine tube by substrate-molecule interactions

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Titanyl phthalocyanine (TiOPc) has received a great attention due to its structural polymorphism and high photoconductivity. Because of the polymorphism, TiOPc crystals in various morphologies have been reported, such as plate-, ribbon-, rod-shape crystals. Here, we report a new tube-shaped TiOPc crystal for the first time. These crystals were obtained in high quality through a simple physical vapor transport (PVT) method. The tube-shaped TiOPc crystals were grown on silicon, silicon oxide and highly ordered pyrolytic graphite (HOPG) substrates. Interestingly, TiOPc crystals were randomly aligned on silicon and silicon oxide substrates, but vertically aligned on a HOPG substrate. We demonstrate that the substrate-molecule interactions affect the crystal alignment, as confirmed by single crystal X-ray diffraction (SCXRD), transmission electron microscopy (TEM), selected area electron diffraction (SAED) data. In general, tube shapes and vertically aligned array properties are advantageous for photonics and electronics because of their large surface area.

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Photoluminescence Properties of New Au(I) Complexes with Dithiocarbamate Ligands

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Department of Chemistry, Chonbuk National University, Korea

A new series of dithiocarbamate ligands, TC-2 (ethyl(pyridin-4-ylmethyl)carbamo-dithioate), was synthesized. Au complexes, $[\text{Au}_2(\text{P-P})(\text{TC-2})]\text{CF}_3\text{CO}_2$ or $\text{Au}_2(\text{P-P})(\text{TC-2})_2$ (P-P = dppm, dppe, dppp), were prepared by the reaction of $[\text{Au}_2(\text{P-P})(\text{CF}_3\text{CO}_2)_2]$ with 1 equiv or 2 equiv of TC-2. These complexes were characterized by FT-IR, NMR, photoluminescence and X-ray crystallography. In $\text{Au}_2(\text{dppe})(\text{TC-2})_2$ crystal structure, TC-2 and P-P ligands bridged two Au(I) ions, each having a transoid coordination geometry and a Au...Au intramolecular distance of 3.0169 (2) Å. The $\text{Au}_2(\text{P-P})(\text{TC-2})_2$ complexes show no luminescence. But $[\text{Au}_2(\text{P-P})(\text{TC-2})](\text{CF}_3\text{CO}_2)_2$ complexes show bright luminescence at $\lambda_{\text{em}} = 535$ nm. The emission properties of Au complexes have relation to alkyl chain length of phosphine ligands. Moreover, anion exchange for 1:1 complexes show luminescence property.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhanced electrical conductivity of Phenazine Radical Crystal through Surface-mediated Recrystallization

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The discovery of the organic metal, TTF-TCNQ, and subsequent enormous research on molecular electronics have drawn attention for the usage of radical molecules as organic conductors with a hope that their unpaired electrons might serve as a charge carrier in radical-based organic materials. However, free radicals are usually very reactive in ambient condition, which is vulnerable to the application in the solid state. That is, it is highly demanded to realize solid state materials possessing radicals. Herein, we report the successfully obtained dihydrophenazinium radical cation crystals (**H₂PNZ^{•+}**) by a simple and fast one-pot photoreaction under Hg irradiation. The obtained crystals showed $\sim 10^{-8}$ S cm⁻¹ electrical conductivity and showed humidity-responsive surface-mediated recrystallization. In the presence of light, the high conducting green radical crystals were formed on the surface of the original **H₂PNZ^{•+}** crystals through the surface-mediated recrystallization process. On the other hand, in the absence of light, neutral state yellow crystals were grown on the surface of the original crystal. Through the single crystal X-ray analyses before and after water exposure to **H₂PNZ^{•+}** crystals revealed that the newly grown high conducting ($\sim 10^{-4}$ S cm⁻¹) green radical crystal had a shorter intercolumnar distance than the original **H₂PNZ^{•+}** crystal. The reduced intercolumnar distance seems to induce a stronger orbital overlap, resulting in enhanced electrical conductivity. Furthermore, the sensitivity to water of **H₂PNZ^{•+}** crystals showed a potential as an electric humidity sensor.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Selective Palladium-Catalyzed Mono Arylation of Ammonia with Tetrameric Sodium tert-Butoxide

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The introduction of aryl groups via the Burkhard Hartwick C-N coupling reaction is of great importance for a fundamental synthesis of numerous drug target molecules and natural products. It is well-known that substitution of the phosphine-containing arene in biarylphosphine ligands can have profound effects of the observed reactivity in catalytic reactions. Herein, we reveal the mechanistic interpretation of chemoselectivity observed in Buchwald's group depending on the difference of substitution in Buchwald ligand. Only the mono-arylated product, aniline, was obtained as the major product from the starting material ammonia at the case of using bulkier ligand L1, whereas the use of other ligand L2 resulted in obtaining the secondary amine product, diphenylamine dominantly. From a simple pKa perspective, it seems natural that an aniline which is more acidic than ammonia can act as a substrate again and easily overcome deprotonation barrier during the catalytic cycle reaching for di-substituted product. Interestingly, according to our DFT calculation, the steric congestion at the complex with L1, which can be considered to maintain proximal configuration to Pd center due to high rotation barrier, has been found to affect the increase of deprotonation barrier. Moreover, the role of tetrameric sodium tert-butoxide that seems to exist highly favorable state in non-polar dioxane solvent is significant to rationalize the reversed chemoselectivity in this work as well as the steric effect of ligand.

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cooperative Effect of an Organic Linker and Open Metal Site on Iodine Chemisorption in a Metal-Organic Framework

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Nuclear power as an alternative to fossil fuels becomes important to meet growing demand for energy owing to their high energy density and less emission of greenhouse gases. However, the release of the radiotoxic radionuclides such as ^{129}I , ^{131}I , ^{137}Cs and ^{90}Sr during the operation of power plants or more seriously during unexpected nuclear accidents could be significantly harmful to human and environment. Recently, therefore, the development of sorbent materials with strong affinity to I_2 has attracted substantial research interest. Metal-organic frameworks (MOFs) have recently emerged as enabling materials for radioactive I_2 sorption owing to their high surface area and designable and tailorable pore properties. In this work, we aim to discover the influence of metal ions and functional groups on the I_2 capture. Several MOFs featured by their isostructures with various organic functional groups and metal ions were chosen as the model materials. The sorption kinetics of the MOF samples were investigated by the use of I_2 dissolved in cyclohexane and I_2 vapor. The further analysis of I_2 @MOFs were employed through single/powder x-ray diffraction (SXR/PXRD) analyses, fourier transform infrared spectrometer (FT-IR), raman spectroscopy, x-ray photoelectron spectroscopy (XPS) and thermogravimetric analyses (TGA).

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Microporous porphyrin network films mimicking velvet worm surface and their enhanced detection abilities of hydrogen chloride and ammonia gases

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This work shows that the functions of microporous organic network materials can be enhanced through engineering of the material structure. Living organisms have adopted intriguing nano/microsized structures for efficient sensing. One of the most studied living organisms for their defensive performance is the velvet worm. The surface of velvet worms consists of villi that are sensitive to the changes of the chemical surroundings. Mimicking the surface structure of velvet worms, we prepared the aligned 1D structure (rod) of microporous porphyrin networks by the Sonogashira coupling of tetrakis(4-ethynylphenyl)porphyrin with 1,4-diiodobenzene in an anodic aluminum oxide plate. The lengths of the 1D structure were controlled to be 1, 2, and 5 μm . The velvet worm surface-like microporous porphyrin networks (Velvet-MPNs) showed higher sensitivities to hydrogen chloride and ammonia gases by up to ~14 and 4.6 times, respectively, compared with a control MPN material without rods and recyclability for the sensing of hydrogen chloride and ammonia.

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Water-Soluble Polymer Entrapment into Superhydrophobic Microporous Organic Networks for the Emission-based Nitrophenol Sensing in Water

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Aggregation-induced emission (AIE) is a versatile phenomenon to be applied for the sensing purpose. Especially, porous materials showing AIE are promising as emission-based sensing materials. In this regard, nano-sized microporous organic network materials bearing tetraphenylethylene moieties were prepared through a growth control using poly(vinylpyrrolidone), PVP. In the synthesis, the PVP was entrapped into the microporous networks. Moreover, the PVP played roles of size control, porosity enhancement, and surface property management. Microporous organic network materials without PVP showed superhydrophobicity with a water contact angle of 151°. In comparison, the microporous organic network with PVP showed excellent water-compatibility. Moreover, due to AIE property of tetraphenylethylene moieties, the microporous organic network showed emission and excellent emission-based sensing of nitrophenols in water with K_{sv} values in the range of $1.26 \times 10^4 \sim 3.37 \times 10^4 \text{ M}^{-1}$. It is noteworthy that the microporous organic network materials in this work used water only as a sensing medium and did not require additional organic solvents to enhance water dispersibility of materials. The microporous organic network materials could be recovered and reused for the sensing at least five times.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Guest-Responsive Metal-Organic Polyhedron for a Colorimetric Sensing Application

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Recently, a growing number of investigators has begun to explore the potential of porous metal-organic materials (MOMs) for sensing applications. So far, the majority of reported sensing materials has been based on luminescence on/off switching of lanthanide ions or aromatic fluorophores upon addition of analytes. Researches of other manners of signal transductions have been relatively less studied. Herein, for the first time, we report a metal-organic polyhedron (MOP) compound which exhibits unusual solvatochromic behavior. The electronic states of the MOP are synergistically altered by organic linkers and metal clusters upon exposure to different organic solvents. The resulting significant color variations of the MOP compounds were successfully observed with naked eyes.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Heterolytic and Homolytic Peroxide Activation Driven by Hydrogen Bonds within Nonheme Copper(II)-Alkylperoxo Complexes

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A room-temperature stable mononuclear nonheme copper(II)-alkylperoxo complex bearing a *N*-(2-ethoxyethanol)-*bis*(2-picolyl)amine ligand (N3O2), [(N3O2)Cu^{II}(OOR)]⁺ (R = cumyl or ^tBu), was prepared and spectroscopically characterized. A combined experimental and theoretical investigations on the reactivity and reaction mechanisms in the phosphorous oxidation and C-H bond activation reactions by copper(II)-alkylperoxo complexes have been conducted. DFT-optimized structure of [(N3O2)Cu^{II}(OOR)]⁺ suggested that hydrogen bonding interaction exist between ethoxyethanol backbone of the N3O2 ligand and either proximal and/or distal oxygen of alkylperoxide moiety; this consequently results in the enhanced stability of the copper(II)-alkylperoxo species. In phosphorous oxidation reaction, heterolytic O-O bond cleavage of copper-alkylperoxo species afforded phosphine oxide and alcohol products. In the C-H bond activation reactions, a rate-limiting hydrogen atom abstraction of xanthene by the putative copper(II)-oxyl radical resulted in the formation of the dimeric copper product and the substrate radical that further underwent the autocatalytic oxidation reactions to form oxygen incorporated product.

Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Phosphatase-Like Activity of A Zinc(II) Complex Bearing Bis(thiosemicarbazone) Ligand: Biomimetic Dephosphorylation Process of Glucose-6-phosphate

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Phosphorylation and dephosphorylation via hydrolytic cleavage of phosphate ester constitute critical conduits for signal transduction, producing the regulation and maintenance of a variety of complicated cellular events. For instance, the tight control of the phosphorylation-dephosphorylation of amino acids residues on the protein surface such as serin, threonine, and tyrosine strongly affects the protein-protein surface interaction by creating a new binding site, inducing the conformational rearrangement and contributing the high-affinity binding via salt bridge and hydrogen bonding. Another important example can be found in the phosphorylation of glucose, resulting in the formation of glucose-6-phosphate since the alterations of glucose metabolism have been revealed to cause diverse disorders including heart disease, diabete and cancer. Therefore, designing small molecules that can modulate the precise control of phosphorylation-dephosphorylation processes has been receiving substantial consideration from the fundamental molecular recognition perspective. In this regard, we synthesized a zinc(II) complex bearing bis(thiosemicarbazone) ligand, which exhibits solvent and pH-dependent geometry. Interestingly, the mononuclear Zn(II) complex displaying distorted octahedral geometry was able to catalyze the dephosphorylation process of glucose-6-phosphate.

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

A Stable Co(III)-Iodosylbenzene Adduct and Effects of Redox-Inactive Metal Ion Binding on Electron Transfer Properties

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High-valent metal–oxygen species are implicated as reactive intermediates in the catalytic oxidation reaction. For example, cobalt(IV)-oxo ($\text{Co}^{\text{IV}}\text{-O}$) species have been proposed as key intermediates in various cobalt-mediated oxidation reactions, such as water oxidation, aromatic and aliphatic C-H bond activation. It has been proposed that redox-inactive metal ions, which act as Lewis acid, are one of the important factors that affect electron-transfer reactivity of high-valent metal-oxygen species. Recently, metal-iodosylbenzene adducts have been considered as reactive intermediate that are capable of conducting various reactions such as oxygen-atom transfer(OAT), hydrogen-atom transfer(HAT) and electron-transfer(ET) reactions. In this regard, we attempt the synthesis and characterization of cobalt-iodosylbenzene adduct bearing $\text{N}_3\text{O}_2(\text{N}_3\text{O}_2 = 2\text{-}(2\text{-}(\text{bis}(\text{pyridin-2-ylmethyl})\text{amino})\text{ethoxy})\text{ethanol})$ ligand, $[(\text{N}_3\text{O}_2)\text{Co}^{\text{III}}(\text{OIPh})]^{2+}$ (**1**), by reacting $[\text{Co}^{\text{II}}(\text{N}_3\text{O}_2)(\text{H}_2\text{O})](\text{ClO}_4)_2$ with excess amount of iodosylbenzene. Interestingly, addition of equimolar of redox-inactive metal ions to solution containing **1** in CH_3CN resulted in the generation of redox-inactive metal ion bound $\text{Co}^{\text{III}}\text{-OIPh}$ complexes, $[(\text{N}_3\text{O}_2)\text{Co}^{\text{III}}(\text{OIPh})]\text{-M}^{\text{n+}}$ ($\text{M}^{\text{n+}} = \text{Ca}^{2+}, \text{Mg}^{2+}, \text{Zn}^{2+}, \text{Y}^{3+}, \text{Al}^{3+}, \text{Sc}^{3+}$) (**1-Mⁿ⁺**). The reactivities of **1** and **1-Mⁿ⁺** were investigated in electron-transfer(ET) reactions. The rates of electron-transfer reactions by **1** were remarkably enhanced by binding of redox-inactive metal ions; this clearly demonstrates the correlation between the reactivity of metal-iodosylbenzene adducts and Lewis acidity of redox-inactive metal ions.

Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

NiO Nanoparticles Embedded in Graphitic Carbon Sheets with Improved Electrochemical Performance as an Anode Material for Lithium-Ion Batteries

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Nickel oxide (NiO) has been attractive as an anode material for lithium ion batteries (LIBs) because of its high theoretical capacity (about 718 mAh g⁻¹), non-toxicity, and low cost. However, NiO suffers from poor cycling stability and rate performance due to rapid particle aggregations, severe volume changes, and low electrical conductivity during the prolonged cycles. To overcome these drawbacks, NiO nanoparticles embedded in graphitic carbon sheets (GCS) were synthesized by polymerization of citric acid and ethylene glycol and carbon template in the presence of a Ni precursor and NaCl. The graphitization of carbon sheets was catalyzed by in-situ formed Ni(0) nanoparticles, improving the conductivity of the carbon sheets. The Ni(0) catalysts were subsequently transformed to NiO nanoparticles. The NiO/GCS composite exhibited the improved electrochemical performances with the reversible capacity of the 1076.2 mAh g⁻¹ after 50 cycle at 0.1 C in the voltage range of 0.01-3.0 V compared to bare NiO (about 285.8 mAh g⁻¹). In addition, the NiO/GCS composite discharged the large reversible capacities of about 743.8 mAh g⁻¹ at 0.5 C and 667 mAh g⁻¹ at 1 C after 100 cycles.

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational study: room temperature olefination of methane with a titanium–carbon multiple bonds

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We report here how methane can be C–H activated, and dehydrocoupled, at room temperature, to ultimately form the olefin $\text{H}_2\text{C}=\text{CHtBu}$ via the addition of a redox-active ligand (L) such as thioxanthen-9-one or 2,2'-bipyridine (bipy) to $(\text{PNP})\text{Ti}=\text{CHtBu}(\text{CH}_3)$ (1). Using both of these exogenous ligand systems, we could trap the elusive “ $(\text{PNP})\text{Ti}(\text{H})$ ” via an insertion reaction into any of these two substrates to afford species of the type $(\text{PNP})\text{Ti}(\text{L})(\text{LH})$. A combination of theoretical and isotopic labeling studies reveal the L ligand to promote the C–C bond step by migration of the methyl moiety in 1 to the α -alkylidene carbon via $(\text{PNP})\text{Ti}\{\text{CH}(\text{CH}_3)\text{tBu}\}(\text{L})$, to eject the olefin and produce a titanium hydride. The latter then is subsequently trapped with an additional equivalent of L. The redox-active ligand plays two critical roles: (i) they accept an electron from the Ti-alkylidene fragment to allow the methyl approaching the alkylidene and (ii) they serve as traps of a formerly titanium(III) hydride generated from olefin elimination. These systems represent the first homogeneous models that can activate methane and selectively dehydrocouple it to an olefin at room temperature.

Poster Presentation : **INOR.P-127**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Bio-inspired Diatom for a motion controlled micromotor and an ultra level sensor applications

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Bio-inspired nanomaterials are of great interest because of their compatibility and less toxicity to nature. Diatoms are one of the classical examples as a bio-inspired material, which are available from marine environment. Moreover, due to their unique structure, and having trace amount of transition metals like SiO₂, Al₂O₃ and Fe₂O₃ endow versatile catalytic as well as sensing activity. In this study, first, we have done selective sensing of hazards toxic aliphatic amines via ‘turn on’ fluorescent mechanism pathway by pyrolyzed diatom with a detection limit of 116 pM. Due to the electron deficient nature of Si⁴⁺, electron rich aliphatic amines can easily bind to diatom resulting in “turn-on” the fluorescence behavior. Moreover, we have also done self-propelled motor machine by pyrolyzed diatom via bubble propulsion by catalytic decomposition of H₂O₂ in the presence of Fe₂O₃ through Fenton catalytic reaction pathway. This natural motor shows an effective motion in the presence of a very low concentration of H₂O₂ (0.8%) as a fuel. Interestingly, the unidirectional motion braking was observed by treatment of EDTA that can stop the movement by chelation with metal. These results illustrate that diatom catalytic micromotors have opened a new era in the field of catalysis and as well as it helped to illustrated sensing field towards wide applications.

Poster Presentation : **INOR.P-128**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Catalytic Cyclic Alkene Oxidation in the Nano Channels of a Copper Silicate Material

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Nanoporous materials related to zeolites and zeotypes are widely employed as its heterogeneous catalysts in the field of partial oxidation research. This study examined the catalytic activity of the copper silicate material SGU-29 for the aerobic partial oxidation of cyclohexene under mild conditions. In particular, the catalytic properties of the CuO_4^{2-} square planar units in SGU-29 were investigated as the active sites for cyclohexene oxidation to generate three main oxidation products (i.e., 2-cyclohexen-1-ol, 2-cyclohexen-1-one, and cyclohexene hydroperoxide). We believe that our study makes a significant contribution to the literature because we demonstrate unequivocally that catalysis occurs only within the inner channels of SGU-29, rather than on the external surface of SGU-29 or within the solvent, and we highlight the special role of the CuO_4^{2-} square planar units in catalysis.

Poster Presentation : **INOR.P-129**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Coordination-Chemistry-Control of Cu(II) Reduction in HKUST-1 Leads to the Enhancement of Water Stability and the Formation of Ship-in-a-Bottle Complex

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Metal-organic frameworks (MOFs) are well-defined nanoporous crystalline materials that can be self-assembled by combining metal ions (or clusters) and multitopic organic ligands via coordination bond. MOFs have attracted significant interests due to their high porosity and large surface area. So they have been employed to many applications such as gas storage, chemical separation, catalysis, and others. For these applications, MOFs have to be chemically stable under the environment which contains water. However, most MOFs are extremely sensitive to water, only a few such as NU-1000, UiO-66, and DUT-51 have shown high resistance to water. For this reason, applying the MOFs for those applications in real industrial system is sometimes very difficult. Thus, finding the new methods to improve the water resistance is an important prerequisite for the expansion of such applications. In general, the water-stable MOFs can be categorized by several approaches such as ligand, multivalent metal, and the protection open metal site (OMS) against water. As reported papers, researchers have trying to enhance the water-stability of MOF by using the various experimental strategies such as metal-ion doping to enhance the metal inertness, ligand functionalization methods to increase the MOFs hydrophobicity. Here, we focus on the discovery of new method to substantially enhance the chemical stability of a MOF, especially water-stability. In this work, we succeeded to control the reduction of Cu(II) metal ion to Cu(I) in HKUST-1 by post synthetic method. And we also find that the modification of metal ion in MOFs makes the consequences that enhancement of water-stability of MOFs.

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Laser-Driven Elimination of Metal-Coordinated Solvents in Metal-Organic Framework.

Hye In Song, Nak Cheon Jeong*

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

Open coordination sites (OCSs) in metal–organic frameworks (MOFs) have shown potential in applications such as molecular separation, sorption, catalysis, and sensing. Thus, the removal of coordinated solvent has been viewed as an essential step that needs to be performed prior to the use of the MOFs in the above applications. To date, a thermal method that is normally performed by applying heat and vacuum has been the most commonly employed activation method despite its negative influence on the structural integrity of the MOFs. Herein, we report that this method can be applied to activate as MOFs in a single-step by showing that, when irradiated with Laser light, this laser energy can efficiently remove the trapped and coordinated solvent molecules from the MOF structure, thereby generating activated MOFs in unprecedentedly short times at atmospheric pressure. These studies will demonstrate not only an effective activation pathway but also effects of solvents on MOF (Solvent polarity or bonding energy). This approach is successful for a broad range of MOFs, including HKUST-1, M-MOF-2(M = Cu, Zn).

Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Rapid Capture and Hydrolysis of a Mustard Gas Simulant in Silver-Ion-exchanged Zeolite Y

Son Yerim, Hyun Sung Kim^{1,*}

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

Sulfur mustard gas, also called HD, is one of the main chemical warfare agents and has claimed thousands of lives and left many more contaminated. The development of functional materials to promptly capture and detoxify sulfur mustard within a few minutes is extremely important to save the lives of the affected people. This has motivated us to explore excellent detoxification systems that can be deployed in the field to rapidly capture and hydrolyze mustard gas in a short time. To that end, we present a silver-ion-exchanged zeolite Y [(Ag⁺)_n@Y, n = 5, 13, 21, 32, 43 and 55] that can rapidly capture mustard gas and its simulant (2-chloroethyl ethyl sulfide, CEES) in ambient conditions to enable the prompt hydrolysis of the CEES captured in its nanopores. The capture and hydrolysis ability of Ag⁺@Y positively correlated with its number of Ag⁺ ions. In addition, 70% of CEES (2.5 mg in 1 mL) was captured by (Ag⁺)₅₅@Y within 20 min at 20 °C in ambient conditions. Moreover, 100% CEES (2.5 mg in 1 mL aqueous ethanol cosolvent) was hydrolyzed in 1 min at 20 °C. The efficiency of (Ag⁺)_n@Y in capturing and hydrolyzing CEES as well as mustard gas is thus a system with high detoxification efficiency for this dangerous chemical warfare agent.

Poster Presentation : **INOR.P-132**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

High Proton Mobility with High Directionality in Isolated Channels of MOF-74

Eun Ji Lee, Nak Cheon Jeong*

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Isolated one-dimensional (1-D) proton channels in a metal organic framework, MOF-74, have been reasonably expected to show highly directional proton conductivity, although no evidence has been provided. As a result of dimensional anisotropy of the channels evenly aligned in c-axis of MOF-74 single crystal, highly directional proton conductivity is demonstrated by using electrochemical impedance spectroscopy. In particular, single crystals treated with sulfuric acid or ammonium hydroxide displays a maximum ~1,200-fold-enhanced c-axis proton conductivity compared to its a-axis conductivity, demonstrating highly directional proton migration through the channels. Very low activation energies (e.g., 0.12 eV) for the c-axis conductivity of MOF-74 also suggest a high proton mobility that arises via Grotthuss proton transfer parallel to the channels.

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Construction of Imidazolium based Metal-organic Framework and Its Dye Sorption Properties

Hyunyong Kim, Eunsung Lee*

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

Building a well-defined porous structure is significant to attract a guest molecule as well as furnishing active linkers to achieve desired functions. There have been various efforts to develop new functional frameworks, but the stability issue always follows in a practical point of view. Herein, we report a highly stable and porous 3D metal-organic framework (MOF) embedding imidazolium groups. Depending on the counteranions of the imidazolium ligand, two distinct MOFs having different dimensions (2D and 3D MOF) were synthesized. 2D MOF constructed by applying bicarbonate anion inhibited three-dimensional growth showed N₂ adsorption with BET results of 330 m²/g. 3D MOF formed by adopting chloride anion of the imidazolium group evolved a 4-fold interpenetrated cube structure. The 3D MOF has high porosity in spite of folded nature of structure with BET results of 1400 m²/g. Interestingly, the multiple π - π interactions of the 3D MOF present unique tolerance toward water for six months and various solvents without decomposition or collapse of the framework. Moreover, since the 3D MOF consists of imidazolium groups, the MOF showed cationic feature with strong adsorption toward anionic guests in aqueous media.

Poster Presentation : **INOR.P-134**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Porous Iridium Cobalt Alloy Nanocages for Efficient Overall Water Splitting Reaction

Jun Kim, Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Since water electrolysis is considered as a practical solution to realize hydrogen economy, developing efficient catalysts is undoubtedly necessary. Despite the low natural abundance and high cost, noble metal (Pt, Ir, Ru) based catalysts have consistently shown unmatched catalytic performances under harsh conditions, thus still nominating themselves as attractive choices. The simple answer to resolve the price issue is to realize a maximum performance with a minimum amount. Herein, we report porous iridium cobalt alloy nanocages for efficient overall water splitting reaction. The design of porous nanocage structure and alloying iridium with cobalt ensures the excellent catalytic performance and durability while minimizing the use of costly iridium.

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of PtPb Nanosponges as Electrocatalysts for the Oxygen Reduction Reaction

Minki Jun, Haneul Jin, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Recently, hydrogen energy is attracting attention as a new energy source because of its advantages over fossil fuels; environment-friendly and efficient. To increase the efficiency of a hydrogen energy system, it is necessary to develop active and stable electrocatalysts. Therefore, various structural and compositional electrocatalysts have been developed. Herein, we report a synthesis of PtPb nanoparticles with the sponge-like porous structure as electrocatalysts for the oxygen reduction reaction (ORR). The prepared PtPb nanocatalysts are expected to show an enhanced performance compared to the commercial Pt/C.

Poster Presentation : **INOR.P-136**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Colloidal synthesis of multiple components nanoparticles based on template-mediated method toward the efficient electrocatalysts

Taekyung Kim, Songa Choi, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nanostructures with multiple compositions and various types of structures containing solid-solid interfaces are important to obtain the multifunctional and synergistic properties. In particular, direct solid-solid interfaces are significant because it is related to enhance the activity of the electrocatalysts, for example, the strain caused by lattice mismatch between interfaces is one of the factors for enhancing activity. However, it is challenging to determine the composition or the order of orientation in the growth of nanostructures. Therefore, the synthetic method for the aforementioned nanoparticles is usually limited, such as top-down templating, surface patterning, or localized deposition. Meanwhile, template-mediated synthesis of nanoparticles is a very efficient method to obtain well-defined colloidal nanocrystals because the template can serve as a platform at which other materials are developed and template components are capable of being released out by dissolution of the template itself. In this research, we suggest the concept of a facile colloidal synthesis of hybrid nanoparticles prepared by the template-mediated method and their possibilities as an efficient electrocatalyst for the hydrogen and oxygen evolution (HER and OER) and oxygen reduction reactions (ORR).

Poster Presentation : **INOR.P-137**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Heterophase nanoframes as active and stable electrocatalysts toward water splitting reaction

Songa Choi, Taekyung Kim, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Iridium-based nanoparticles are widely used electrocatalysts for oxygen evolution reaction (OER) and platinum is also the most commonly utilized toward hydrogen evolution reaction (HER) due to its high activity. From a structural point of view, nanoframes have the intrinsic large surface area to enhance catalytic activity because their hollow structures have many active sites as electrocatalysts for water splitting. Herein, we report the synthesis of heterophase IrNi edges- PtNi axes of one nanoframe as an active and stable electrocatalyst for overall water splitting. The IrNi/PtNi heterophase-nanoframes could be synthesized by controlling the differences in decomposition kinetics of each metal precursor and would be expected to have enhanced activity and stability for overall water splitting in acidic media.

Poster Presentation : **INOR.P-138**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Polymetallic Catalyst bearing Rare Earth Metal For Cycloaddition of CO₂ with epoxides

Na Ru Kang, Jin Seong Oh, Jungseok Heo^{1,*}

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The reduction on carbon dioxide emissions is being studied around the world as a way to solve environmental problems such as global warming. In particular, research is actively conducted to utilize carbon dioxide as a useful resource based on the building block [1-3]. Among them, the cyclic carbonate and polycarbonate, which are produced through the copolymerization of carbon dioxide and epoxide, are widely used in eco-friendly plastics [4] and electrolytes of lithium ion batteries [5]. We previously reported Zn-complex catalyst that increased carbon dioxide accessibility through ligand with four metal sites. This time, we present a catalyst that is expected to be more efficient through switching metal ions with cerium ions, the most common rare earth metals. Cerium is widely used for the conversion of carbon dioxide in the form of oxide and can form bonds with various forms of carbonate, such as monodentate and bidentate [6], so a good efficiency catalyst can be expected. In the poster session, we will present details on catalytic properties of the new catalyst.

Poster Presentation : **INOR.P-139**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of asymmetric bending 2D metal chalcogenide heteronanoplates via modulation of the surface strain

Jisol Park, Sunghyun Lim¹, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

¹Chemistry, Korea University, Korea

Modulation of the surface strain within the nanostructures has been intensively investigated due to it affects the electrocatalytic performance by changing the electronic state at the surface atoms. Hetero-interfaces driven from the two kinds of materials induce the lattice mismatch, inducing the high electrocatalytic activity. However, the control of surface strain via synthesis of asymmetric bending 2D metal chalcogenide nanoplates has been rarely reported. Herein, we reported that the synthesis of Rh-based bending Janus nanoplates by controlling the reaction kinetics, having high surface strain compared to conventional 2D flat nanoplates. They also exhibit enhanced electrocatalytic performance toward hydrogen evolution reaction (HER) and they could be changed depending on the degree of bending.

Poster Presentation : **INOR.P-140**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Detection of Phosphate anion through Membrane Electrode based on Zn-complex.

Jin Seong Oh, Na Ru Kang, Jungseok Heo^{1,*}

Chemistry, Chungnam National University, Korea

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Jinseong Oh, Naru Kang, and Jungseok Heo*Department of Chemistry, Chungnam National University, Daejeon 305-764, South KoreaElectronics and Telecommunications Research InstituteE-mail: jungseokheo@cnu.ac.kr As the Importance of anionic species increase in biology, catalysts and the environment, we are interested in developing molecules that can selectively recognize and detect these negatively charged ions. The development of receptors and sensors for anions in nature is emerging as an important research area [1]. Sensors for various ions have been studied, and here we have synthesized a phosphate sensitive zinc complex that **has good selectivity** for phosphate anion. Though many reported phosphate sensors include Zinc and a 2, 2'-dipicolylamine arm [2], there are few reports, to the best of our knowledge, of Zinc based phosphate sensing complexes derived from a 2-picolylamine or L-lysine hydrochloride. 2-Hydroxybenzene-1,3,5-tricarbaldehyde and 2-picolylamine(or L-lysine hydrochloride) were synthesized to a ligand having two metal sites and then synthesized with a Zn-compound to create a dinuclear Zinc complex. And we made this into a membrane type and combined it with electrode to measure the amount of sensed phosphate anion [3]. References1.(a) Brzo'zka,Z. In "Comprehensive Supramolecular Chemistry"; Atwood, J. L., Davies, J.E.D., MacnNicol, D.D., Vögtle, F., Suslick, K, S., Eds.; Pergamon: Oxford, **1996**; pp 187-212 (b) "Chemosensors of Ion and Molecular Recognition"; Desvergne,J.-P., Czarnik, A. W., Eds.; Kluwer: Dordrecht, **1997**; Vol 492.2.(a) "Highly effective fluorescent and colorimetric sensors for pyrophosphate over H₂PO₄ in 100% aqueous solution". Jang, Y. J.; Jun, E. J.; Lee, Y.J.; Kim, Y. S.; Kim, J. S.; Yoon, J. J. *Org. Chem.* **2005**, 70, 9603. (b) "Bis(Dpa-ZnII) Appended Xanthone: Excitation Ratiometric Chemosensor for Phosphate Anions". Ojida, A.; Nonaka, H.; Miyahara, Y.; Tamaru, S.-I.; Sada, K.; Hamachi, I. *Angew. Chem., Int. Ed.* **2006**, 45, 5518; for CTP3 sensing, see:3."Phosphate-selective polymer membrane electrode", Scott A. Glazer, and Mark A. Arnold, *Anal. Chem.*, **1998**, 60 (22), pp 2540-2542.

Poster Presentation : **INOR.P-141**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of bent copper sulfide nanoplates via specific cation exchange

Sunghyun Lim, Taehyun Kwon¹, Kwangyeol Lee^{1,*}

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There are emerging attentions about nanostructured semiconductors due to their unique physical properties depending on their size, phase, and morphology. Therefore, synthetic strategy to prepare semiconductor nanoparticles with well-defined morphology and size have received enormous interests in the past few decades. Also, more advanced nanostructure design could be achieved by exploiting ion exchange, hetero-epitaxial growth, galvanic exchange, etc. Among these methods, ion exchange reaction is emerging as a powerful synthetic pathway for synthesizing one targeted material. Herein, we report the synthetic strategy to prepare bent copper-based sulfide nanoplates via site-specific cation exchange method.

Poster Presentation : **INOR.P-142**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Diastereoselective Intramolecular Rhodium-Catalyzed [(3+2+2)] Carbocyclization Reactions with Tethered Alkynylidenecyclopropanes: Synthesis of the Tremulane Sesquiterpene Natural Products

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The development of a highly diastereoselective intramolecular rhodium-catalyzed [(3+2+2)] carbocyclization reaction of allyl-tethered alkynylidenecyclopropanes (ACPs) is described. This work illustrates that the stereoelectronic nature of the phosphite ligand dramatically impacts the level of stereocontrol in the facial addition of the tethered alkene to the metallacycle to afford the syn-diastereoisomer. Density functional theory(DFT) study is done to investigate the origin of diastereoselectivity.

Poster Presentation : **INOR.P-143**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of Crystalline Pd₁₃Cu₃S₇ Nanodisc via Cation Exchange on Metastable Copper Sulfide Template toward Hydrogen Evolution Reaction

Haneul Jin, Yongju Hong, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Hydrogen production via water electrolysis is essential in hydrogen energy cycle and finding an optimum catalyst is of great interest in hydrogen evolution reaction (HER). Herein, we synthesized crystalline Pd₁₃Cu₃S₇ nanodisc via partial cation exchange using Cu_{1.81}S nanoplate as a template. In the synthetic process, metastable Cu_{1.81}S became a great template because of the leachable characteristics of Cu and the unique crystal structure of copper sulfide. We also obtained an amorphous PdCuS nanoplate by a kinetic control of the synthetic reaction. As-synthesized Pd₁₃Cu₃S₇ nanodisc showed 6 times higher mass activity (per Pd) and 14 times higher specific activity than amorphous PdCuS nanodisc toward HER in the acidic electrolyte, which indicated the importance of crystallinity for electrolytic hydrogen evolution on Pd₁₃Cu₃S₇ nanodisc.

Poster Presentation : **INOR.P-144**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Edge-reinforced hollow rhodium phosphosulfide: a highly active and robust electrocatalyst toward hydrogen evolution reaction

Yongju Hong, Haneul Jin, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

High-performance and robust metal electrocatalysts toward hydrogen evolution reaction (HER) are essential to accelerate the realization of hydrogen energy that could replace fossil fuels in the future. The transition metal phosphides (TMPs) have been known for the great catalytic activity but with unsatisfactory stability in HER. However, the theoretical and experimental studies have proved that the partial ion exchanges that tune the electronic structures of the active sites lead great enhancement in both the catalytic activity and rigidity. Recently, we found a facile route to form the tire-like rhodium phosphosulfide nanocatalysts through post-phosphidation. The Kirkendall effect and the difference in the stoichiometry of metal phosphides and sulfides induced hollow core and rough surface, which could contribute the excellent electrocatalytic performance toward HER.

Poster Presentation : **INOR.P-145**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

The synthesis of Cu₂O templates for CdS and CdSe nanocages

Jinwhan Joo, Ye Ji Park¹, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

¹*Korea University, Korea*

Semiconductor nanostructures have received a great attention due to their size-tunable optical properties and have various applications in catalysis, laser, and solar cell. The optical properties of the semiconductor are tightly coupled with the morphologies of the nanostructures. Herein, we developed a sequential anion exchange, chemical etching, and cation exchange strategy for preparing CdS and CdSe nanocages. We first synthesize cubic and rhombic dodecahedron Cu₂O nanoparticles for templates through the wet-chemical reaction. The sequential anion exchange and chemical etching of Cu₂O templates lead to the formation of CdS and CdSe nanocages. We finally report the unique optical properties of CdS and CdSe nanocages from the structural difference between cubic and rhombic dodecahedron CdS nanocages as well as composition difference between sulfur and selenium.

Poster Presentation : **INOR.P-146**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Ligand-free synthetic method of $\text{Ag}_x\text{Cu}_{1-x}\text{S}$ alloy nanoparticles

Jinwhan Joo, Ye Ji Park¹, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

¹*Korea University, Korea*

Electrocatalytic reactions, including oxygen evolution reaction, hydrogen evolution reaction, and CO_2 reduction reaction, plays a key role to the hydrogen society and environmental impact of CO_2 . Although, the nano-scale electrocatalysts have been achieved significant progresses in the past years, several undesirable issues remain in nano-scale electrocatalysts. First, the large size and polydispersity of the reported nanoparticles hamper its real utilizations. Second, introducing ligand remains a necessary step for the preparation of well-defined nanoparticles, which restrict the exposure of active site and thus decreases the catalytic performances. Herein, we report a highly dispersive $\text{Ag}_x\text{Cu}_{1-x}\text{S}$ alloy nanoparticles by using a facile, ligand-free synthetic method. The elemental composition can be easily controlled through adjusting the ratio of metal precursors.

Poster Presentation : **INOR.P-147**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Ir-based ternary octahedral nanocages by 3d-transition metal doping for efficient electrocatalyst for the oxygen evolution reaction

Taehyun Kwon, Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nanoparticles with hollow interior such as nanocages, nanoframes, etc. have received enormous attention due to their high electrocatalytic activity toward water splitting. In particular, iridium(Ir)-based hollow nanostructures are widely used as electrocatalyst for the oxygen evolution reaction (OER) under acidic condition, which is rate determining step for overall water splitting reaction. We have previously reported the introduction of cobalt(Co) during the synthesis of IrCu octahedral nanocrystal as a dopant, which enabled the formation of ternary Co-doped IrCu octahedral nanocages as an efficient oxygen evolution catalyst. In this presentation, the similar role of other 3d-transition metal elements like Co, which directs the formation of ternary IrCu nanocages, will be presented. Also, the relations between the dopant element and the OER performance will be presented.

Poster Presentation : **INOR.P-148**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of Yttrium Based 1D Metal-Organic Cage Framework and Its Post-Exchange of Internal Yttrium Cluster Inside the Cage with Alkali Metal Ions

Nakeun Ko, Eunsung Lee*, Kimoon Kim*

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

Metal-organic frameworks (MOFs) are composed of well-defined metal clusters and organic linkers, which afford various structures and capability to functionalize the framework for enhanced catalyst, gas storage, and separation properties. Organic linkers with an imidazolium functional group were studied for specific application of proton conduction and N-heterocyclic carbene (NHC) chemistry. Through a solvothermal reaction of yttrium cation with L = 1,3-bis(3-carboxyphenyl)imidazolium chloride, 1D metal-organic cage framework was synthesized and characterized by single-crystal X-ray diffraction analysis. The yttrium based MOF (YMOF) has a 1D chain structure with octa-imidazolium cages. In the cage, a Y₄ cluster locates and connects the 1D chain by the formates. YMOF can be further modified for removal of the Y₄ cluster for improving the porosity of YMOF and subsequent refilling of the void volume with alkali metal ions. The detailed study will be presented.

Poster Presentation : **INOR.P-149**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Nanoscale mixed-ligand MOFs (NMLM) showed highly visible-light-driven photocatalytic activities for Rh B degradation

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Metal-organic frameworks (MOFs), consisting of organic ligands and inorganic secondary building unit (SBU), have emerged as a potential alternative to a conventional photocatalyst because of their ultra-high surface area, rigid structure, and tailorable functionality. But these new materials have challenges still remain because of hole-electron's rapid charge recombination and narrow absorption region. Recently, porphyrin and zirconium based MOF, PCN-222, was used to photocatalyst in which charge recombination was retarded by effective charge transfer between metal cluster and ligands.¹ However, inferior solar spectrum coverage of PCN-222 still needs to be improved. In this study, the nanoscale mixed-ligand MOFs (NMLM) was successfully synthesized for enhancing the photocatalytic activity. NMLM was formed by mixing pyrene and porphyrin and showed high photodegradation efficiency of Rhodamine B (Rh B) due to the complementary absorption properties and efficient energy transfer between pyrene and porphyrin unit in the NMLM. The present study provides a new way for using the photoactive MOFs and efficient system for organic pollutant degradation.1. C. Xu, H. Liu, D. Li, J. Su, H. Jiang, Direct evidence of charge separation in a metal-organic framework: efficient and selective photocatalytic oxidative coupling of amines via charge and energy transfer, *Chem. Sci.* 9 (2018) 3152-3158.

Poster Presentation : **INOR.P-150**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Polymorphs of sodalite-like zeolitic imidazolate frameworks exhibiting different porosity

Kyungkyou Noh, Jisu Lee¹, You Jin Oh¹, Jaheon Kim^{1,*}

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¹Department of Chemistry, Soongsil University, Korea

Two polymorphous zeolitic imidazolate frameworks (ZIFs) (termed α -ZIF and β -ZIF) were synthesized respectively by the solvothermal reactions between zinc ion and 2-nitroimidazole employing different solvent conditions. Crystal structures showed that both ZIFs had the same composition and adopted the same sodalite-like topology with different linker orientations in the six-membered rings of sodalite-cages. This structural difference gave rise to different N₂ adsorption properties, and phase transition behaviors as well. In particular, the β -ZIF adsorbed almost three times more gaseous benzene than the α -ZIF.

Poster Presentation : **INOR.P-151**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Enzyme-mimicking metal-organic frameworks

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To make Fe- and Cr-MIL-101 metal-organic frameworks (MOFs) mimic the catalytic functions of enzymes, the MOFs were functionalized with various amino acids. Two approaches have been used for the functionalization. First, amino acids were covalently attached to the functional groups of the framework ligands using sequential coupling reactions. In the second method, space molecules were attached before introduction of amino acids. The amino acids-functionalized MOFs were applied to the decarboxylation reactions of organic substrates.

Poster Presentation : **INOR.P-152**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Pyrene-Based Supramolecular Polymer in Aqueous Solution

Sojeong Heo, Heekyoung Choi, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Noncovalent interactions such as hydrogen bonding, π - π stacking, dipole-dipole interaction, and Van der Waals forces produce thermodynamically ordered associations of self-organized materials. The pyrene excimer is very sensitive to the distance between and the geometry of two close pyrene units. So pyrene units have been used for monitoring conformational changes and interactions in supramolecular assembly. The functional building block **1** composed of pyrene and bipyridine moieties was synthesized by multi-steps to prepare supramolecular polymer. The supramolecular polymer **1** was prepared by compound **1** in different composition of DMSO/water. The supramolecular polymer **1** was characterized by photoluminescence (PL), circular dichroism (CD), atomic force microscopy (AFM). The sky blue emission of supramolecular polymer **1** showed at 470 nm in DMSO/water (50:50 v/v) whereas the yellow emission of supramolecular polymer **1** showed at 520 nm in DMSO/water (99:1 v/v). Interestingly, the blue emission exhibited CD signal, indicating that building blocks **1** were orientated to the left-handed helical direction. According to AFM observations, the supramolecular polymer **1** formed in DMSO/water (50:50 v/v) showed the left-handed helical fibers and the supramolecular polymer **1** formed in DMSO/water (99:1 v/v) showed the linear aggregates. In this workshop, I will detail present unusual emission according to the solvent composition.

Poster Presentation : **INOR.P-153**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

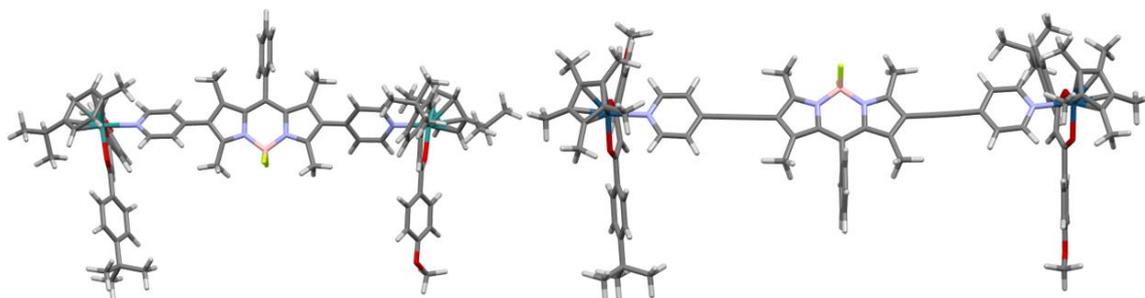
Bodipy based Ru(II) and Ir(III) complexes of Avobenzone

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The use of biologically active organic molecules for the synthesis of metal based complexes is an alternative strategy for the development of anticancer drugs to minimise its unwanted harmful side effects. On the other hand, boron-dipyrromethene, commonly known as bodipy, are well known fluorescent molecules used for several important applications including biological labelling.¹ Herein, we combine avobenzone, a sunscreen material, with bodipy to synthesize new Ru(II) and Ir(III) metal based avobenzone-bodipy supramolecules.² The new complexes were fully characterized by different analytical techniques and their structures were rationalized using density functional theory calculations and further applied for biological studies. The complexes were found to be highly active in different cancer cell lines with half maximal inhibitory concentration (IC₅₀) between 1-5 μ M and their activity is comparable to that of chemotherapy drug doxorubicin. Further studies showed that the complexes also exhibit good DNA binding properties.



Poster Presentation : **INOR.P-154**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Helicity Control of the Supramolecular Organometallic Gel

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We demonstrate the change of helical directions and morphologies in supramolecular gels according to the concentration of organometallic compound. We synthesized two terpyridine derivatives (**tpy-1**, **tpy-Pt^{II}**) as gelators for a supramolecular gel. The mixtures of **tpy-1** and **tpy-Pt^{II}** with various ratios were gelled in DMSO/H₂O. The gelations were presumably mediated by the Pt–Pt and π – π stacking interactions. The CD spectra of the supramolecular organometallic gel formed with small ratio of **tpy-Pt^{II}** showed left helicity that originates from the enantiomeric L-form alanine moiety embedded in the gelators. However, the left-handed helicity was inverted to form right-handed helicity upon addition of more **tpy-Pt^{II}**, indicating that the additionally added organometallic compound greatly affected the intermolecular interactions in the supramolecular organometallic gel network, influencing the helicity at the supramolecular level. More interestingly, morphology observation in SEM images more clearly exhibited that the helicity of supramolecular nanofibers was inverted from left to right with increasing the ratio of **tpy-Pt^{II}**. The results demonstrate that the helicity inversion and morphology change are mainly mediated by increase of the metal to metal interactions between the organometallic molecules.

Poster Presentation : **INOR.P-155**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Single-atom iron implanted nitrogen doped porous carbon for efficient oxygen reduction reaction in alkaline media

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Recently, exhaustion of fossil fuel resources and related environmental problems have prompted demand for renewable and green energy. Although fuel cells are considered a promising clean energy technology, platinum, as a catalyst in the cathode in fuel cells, has the problems such as high cost, scarcity, and low stability. Therefore, it is necessary to develop a non-precious metal catalyst having a low cost and high efficiency in order to replace platinum. In this study, we synthesized atomically dispersed iron-nitrogen doped porous carbon catalysts derived from iron-porphyrin encapsulated ZIF-8 which is embedded in carbon black. The synthesized catalyst is characterized by various technique including BET, XRD, Raman, XPS, SEM, and TEM. Characterization revealed that the single-atom Fe-N₄ active sites is uniformly dispersed. Synthesized catalysts exhibit outstanding performance and excellent durability in alkaline media.

Poster Presentation : **INOR.P-156**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Colorimetric detection of Hg²⁺ in water via metal-organic frameworks (MOFs)

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Metal-organic frameworks (MOFs), constructing via coordination bond between inorganic secondary building units (SBU) and organic building block, have emerged as the innovative porous materials. Enormous surface areas, versatile tunability, confined pore-size and regularity of MOFs enable us to demonstrate the various applications including gas storage, separation, sensing, drug delivery, electrocatalysis, and catalysis. Among them, use of metal-organic frameworks by fluorescence detection method are actively being carried out. Since MOFs are excellent in stability and have the advantage of using various organic ligands, it is easy to detect heavy metal ion in aqueous solution through MOFs with proper ligands. In this study, thiol-functionalized MOF, SALI-MAA-3eq, was synthesized by incorporating mercaptoacetic acid into stable, Zr-based MOF, NU-1000 via solvent-assisted ligand incorporation (SALI) approach. SALI-MAA-3eq was fully characterized by common analytical techniques and further applied for sensing applications. SALI-MAA-3eq was found to selectively detect Hg²⁺ over a range of metal ions in water environment which has been confirmed by X-ray photoelectron spectroscopy (XPS) studies and fluorescence.

Poster Presentation : **INOR.P-157**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Surfactant-free electrochemical synthesis of metallic nanoparticles *via* stochastic collisions of aqueous nanodroplet reactors

Young Eun Jeun, Hyun Seo Ahn*

Department of Chemistry, Yonsei University, Korea

Stochastic collisions of aqueous nanodroplets (AnDs) on a microelectrode were observed *in situ* by electrochemistry. Reduction of Cu^{2+} ions enclosed in the reacting AnDs resulted in surfactant-free synthesis of copper nanoparticles on the electrode surface. The particle size distribution was reasonably controllable by the modulation of electrode voltage. The versatility of the synthetic method was established by its application in synthesizing nanoparticles of silver and cobalt oxyhydroxide.

Poster Presentation : **INOR.P-158**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Investigation of Site-Selective Electron Transfer with Low Energy Excitation in Ir(III)-Pt(II) Bimetallic Complexes

Hyun Wook Cha, So-Yoen Kim, Chul Hoon Kim*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Photodynamic behaviors in Ir(III)-Pt(II) bimetallic complex were differentiated by changing bridging ligand that connect the two metal centers: twisted co-planar (2,3-bis(2-pyridyl)pyrazine, **dpp**) and fully-planar moiety (4,7-phenanthroline-5,6:5',6'-pyrazine, **ppz**). In particular, low-energy excitation (530 nm) makes a clear distinction between photo-induced electron transfer (PET) and hole transfer (PHT) after photo-excitation of bimetallic complex that otherwise would not be able to be achieved under high excitation beam energy. The PHT process was only observed in (dfppy)₂Ir-dpp-PtCl₂. The fast quenching process occurring in the Ir-³MLCT state of (dfppy)₂Ir-dpp-PtCl₂ was further investigated by time-resolved photoluminescence (TRPL) and femtosecond transient absorption (TA) spectroscopy.

Poster Presentation : **INOR.P-159**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Porous Polymers Derived from Ti-Oxo Clusters

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Recently, porous polymers have attracted considerable research attention for their diverse applications such as gas storage, separation, and sensors. In general, however, the absence of photoactive sites limits them from photocatalytic applications. In this research, we tried to overcome this weakness by the use of Ti-oxo clusters as monomers of porous polymers. As a result, new types of the porous polymers consisting of photo-active Ti-oxo clusters were successfully synthesized and their photocatalytic activities are carefully examined. Interestingly, the polymers possess hierarchically porous structures ranged from micro- to macropores, which will be beneficial for fast kinetics in guest molecule adsorption or catalytic applications. Moreover, they exhibit high air and moisture stability due to their covalent bond-based networks.

Poster Presentation : **INOR.P-160**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

New Zr-MOFs composed of hetero-linkers with an *fcu* topology via post-synthetic ligand insertions

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

The synthesis of metal-organic frameworks (MOFs) composed of hetero-linkers is important for tuning framework properties. Despite tremendous endeavor, it is still challenging to synthesize Zr-MOFs with hetero-linkers of different lengths. Recently, preparations of Zr-MOFs of 12-connectivity that contain hetero-linkers were reported via sequential insertions of additional linkers into an 8-c Zr-MOF, PCN-700. Since the Zr clusters, $[\text{Zr}_6\text{O}_4(\text{OH})_4(\text{COO})_{12}]$ SBUs, in PCN-700 are alternating in two different orientations, the 12-c MOF obtained is not of an **fcu** topology. Here we report the preparation of a series of new Zr-MOFs with an **fcu** topology via post-synthetic ligand insertions using hetero-linkers of different lengths. A solvothermal reaction of ZrOCl_2 and 2,6-naphthalene dicarboxylic acid (H_2NDC) with coplanar conformation of the carboxylate residues produced a new flexible Zr-based MOF, $[\text{Zr}_6\text{O}_4(\text{OH})_4(\text{NDC})_4(\text{H}_2\text{O})_8](\text{monoacid})_4$ (**ZRN**), with an 8-c **bcu** topology. A series of new Zr-MOFs with an **fcu** topology can be obtained via simple soaking method. When **ZRN** crystals were put into a solution of functionalized 1,4-benzene dicarboxylic acid (H_2XBDC), even though the shortest distance between the closest neighboring Zr-SBUs with potential linkage sites in **ZRN** is longer than the length of XBDC derivative but the XBDC linkers are inserted into the remaining potential linkage sites to form a new framework with a 12-c **fcu** topology. Single crystal structure analyses confirmed the different binding modes of the inserted linkers between $[\text{Zr}_6\text{O}_4(\text{OH})_4(\text{COO})_{12}]$ SBUs depending on the functional groups of the inserted hetero-linkers

Poster Presentation : **INOR.P-161**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Quinolinol-based Al/Triarylborane Dyad Assembly: Alteration of Electronic Transition States Mediated by Fluoride Anion Binding

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In this study, we synthesized quinolinol-ligand (2-methylquinolin-8-ol, q)-based aluminum complexes with phenyl (**D1**), biphenyl (**D2**), and naphthyl (**D3**)-bridged triarylboranes, and employed them as organometallic chemosensors for sensing mediated by fluoride anions. In addition, these dyad complexes were fully characterized by multinuclear nuclear magnetic resonance (NMR) spectroscopy and elemental analysis. UV/Vis titration experiments examining the association of **D1**, **D2**, and **D3** with fluoride demonstrated that the dyad complexes associated in a 1:1 binding stoichiometry in tetrahydrofuran THF, with binding constants (K) in the range of $2.7 \sim 6.6 \times 10^4 \text{ M}^{-1}$. Moreover, these dyad complexes showed a ratiometrically decreasing fluorescence response in PL titration experiments upon binding of fluoride to the borane moiety, thereby giving rise to a turn-off chemosensor for detection of fluoride anions. It could be postulated that these turn-off properties were caused by the interruption of the intramolecular charge-transfer (ICT) transition between the q₂Al part and the bridged phenoxy groups. Furthermore, the theoretical calculation results for the dyad complexes and these fluoride adducts clearly indicate that the ICT transition between the q₂Al and bridged phenoxy groups of the complexes could be interrupted by the binding of fluoride to borane.

Poster Presentation : **INOR.P-162**

Inorganic Chemistry

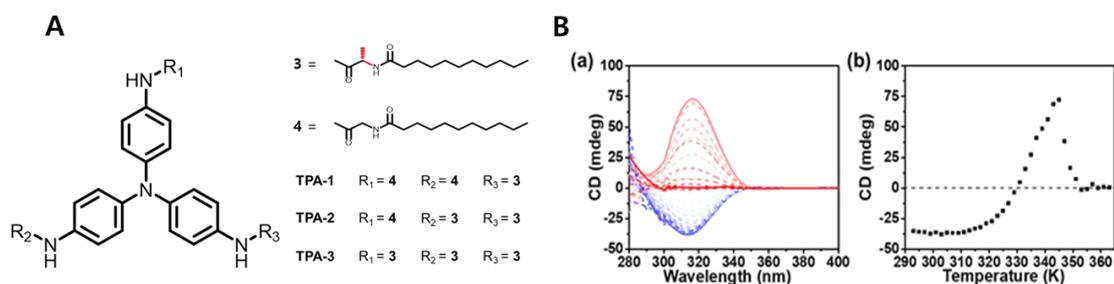
Grand Ballroom, FRI 11:00~12:30

Unexpected Helical Inversion of Asymmetric Triphenylamine-Based Supramolecular Polymers

Misun Go, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We describe unique helicity inversion of supramolecular polymers based on triphenylamine (TPAs) bearing different number of alanine and glycine moieties by change of temperature. Despite chiral branching differences, three TPAs form helical supramolecular polymers by a typical nucleation-elongation model characteristic of a cooperative assembly. Temperature-dependent circular dichroism (CD) observations revealed that supramolecular polymers **TPA-1** and **TPA-2** showed the peculiar helical inversion during heating. Self-assembled **TPA-1** and **TPA-2** showed the left-handed helicity (M-type) at lower temperature whereas **TPA-1** and **TPA-2** showed the right-handed helicity (P-type) at higher temperature. AFM images showed that the self-assembled **TPA-1** and **TPA-2** exhibited co-existence of both the left- and the right-handed helical fiber at lower and higher temperatures. However, the left-handed helical fiber existed as a major product at lower temperature was converted to the right-handed helical fiber at higher temperature. In contrast, the self-assembled **TPA-3** showed an ambiguous left-handed helical structure with long helical pitch.



Poster Presentation : **INOR.P-163**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cyano-stilbene-based fluorescent probe for the detection of hydroxyl radicals in pure aqueous solution and living cell

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Gyeongsang National University, Korea

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

Since high selective and sensitive detection of hydroxyl radicals in living cells is challenge for evaluating the role that hydroxyl radicals plays in the biological system, new cyanostilbene-based fluorescent probe **1** for hydroxyl radicals was synthesized. The fluorescent probe **1** shows strong green emission upon the addition of hydroxyl radicals in aqueous solution. In contrast, negligible changes in the emission were noted upon addition of other reduced oxygen species (ROS). The probe **1** exhibited high sensitivity with low detection limit to $\sim 1.25 \times 10^{-9}$ M. In particular, probe **1** showed low cytotoxicity, and was successfully applied to bioimaging of hydroxyl radicals in the live cell. These findings indicate that new probe **1** has great potential to bioimaging in vitro and in vivo systems.

Poster Presentation : **INOR.P-164**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Electrophilic *N*-Heterocyclic Carbene Azido Cation

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The stabilization of homoatomic main group element fragments by the neutral, two electron donors such as carbenes is the recent renaissance in p-block main group chemistry. Our group successfully prepared the cationic N₃ species featuring N-heterocyclic carbene. Herein, we present a novel electrophilic reagent, *N*-heterocyclic carbene azido cation and its reactivities toward various nucleophiles including hydroxide, azide, carbene, and phosphine. Experimental descriptions and theoretical studies of each reaction will be shown.

Poster Presentation : **INOR.P-165**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Modeling gas adsorption properties in triangular metal-organic frameworks with defects

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School of Chemical and Biomolecular Engineering, Pusan National University, Korea

Defects in metal-organic frameworks (MOFs) have been received tremendous attention during the past few years because the introduction of defects in MOFs could introduce new active sites in MOFs for gas separation and catalysis. One type of defects is linker defects, in which the linkers connecting the inorganic nodes is removed during the activation process which leaves open metal sites that can be used for selective adsorption or catalysis. Depending on the solvents used during the synthesis, the solvent molecules occupy the open metal sites created from linker defects and provide additional interaction sites for gas adsorption. However, less is known about the impact of solvents in the gas adsorption properties. In this work, we used a combination of molecular modeling techniques and macroscopic breakthrough simulations to model the adsorption characteristics of triangular MOF, which has been received much attention for its unprecedented separation capability of hexane isomers. We have created different degree of defect models for triangular MOFs, from 5 - 20 %, on the basis of solvents that has been used in the experiments. Configurational-biased grand canonical Monte Carlo (CB-GCMC) simulations are carried out to test hexane isomer selectivity and precombustion CO₂/H₂ separation capability at the operating conditions. Breakthrough simulations are subsequently carried out to elucidate the impact of defects on different gas separation applications.

Poster Presentation : **INOR.P-166**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

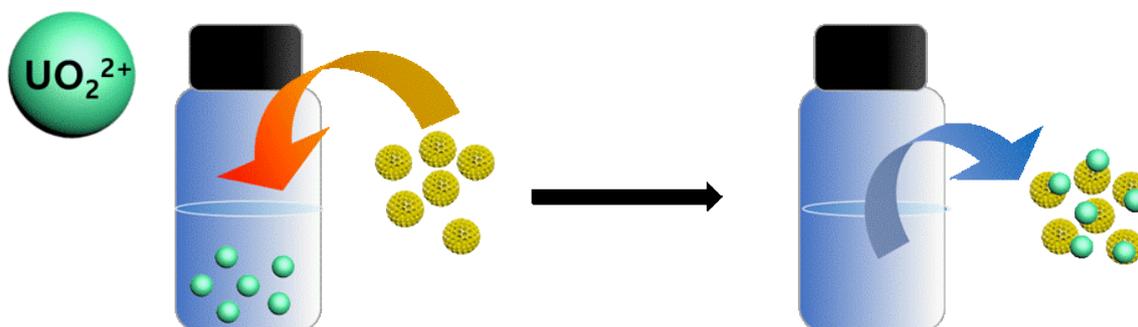
Highly selective chromogenic probe and adsorbent for uranyl ion in aqueous solution

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Department of Chemistry, Gyeongsang National University, Korea

¹Department of Chemistry, Gyeongsang National University, Korea

Uranium is an important natural radionuclide, and widely used in civilian and military, and can cause several health problems. Thus, the development of chemical probes for uranium is extremely important for the medical and industrial fields. Herein, we describe the chemosensing ability of a salicyldeazine derivative (**1**) as fluorogenic probe for uranyl ions. The strong luminescence of ligand **1** at 550 nm was largely quenched upon addition of UO_2^{2+} , but not any other metal ions. This quenching effect was due to complex formation between **1** and UO_2^{2+} ion. Ligand **1** showed good a liner range of 50-500 ppb UO_2^{2+} with a detect limit of 10.2 ppb at pH 7. In contrast, no significant luminescence change in **1** was observed upon addition of other metal ions. In particular, the mesoporous silica (**MS-1**) embedded **1** was prepared by sol-gel polymerization. The adsorption capacity of **MS-1** was evaluated upon addition of UO_2^{2+} . In this conference, we will present on chemical sensing ability of **1** and the adsorption capacity of **MS-1**.



Poster Presentation : **INOR.P-167**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Solvent-driven single crystal to single crystal (SCSC) transformation from 0D to 1D in azamacrocyclic complex

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Division of Daegu, Korea Institute of Science and Technology Informat, Korea

¹Beam Operation Team, Pohang Accelerator Laboratory, Korea

Single crystal to single crystal (SCSC) transformations in coordination compounds are important phenomena and are fascinating because they lead to the formation of unusual compounds which cannot be designed by general synthetic process or cannot be proposed molecular structures. Whereas the phenomenon of SCSC in coordination compound has well noticed long ago, the conversions of coordination compounds from 0D to 1D or 1D to 2D or 2D to 3D are still rare. To investigate the SCSC transformation of azamacrocyclic complex, we synthesized the new copper(II) azamacrocyclic complex with butyl pendent groups and 2,7-naphthalenedicarboxylic acid (2,7-NDC) ligand. When a drop of MeOH was added to the violet crystal of 0D discrete copper(II) complex, $[(\text{Cu}(\text{C}_{16}\text{H}_{38}\text{N}_6)(\text{H}_2\text{O})_2)][2,7\text{-NDC}]$ (**1**), it immediately transformed to a pink crystal 1D coordination polymer, $[(\text{Cu}(\text{C}_{16}\text{H}_{38}\text{N}_6)(2,7\text{-NDC}))_n]$ (**2**). Here, we will elucidate the preparation, crystal structures of SCSC transformation and interesting solvent-induced PXRD analysis.

Poster Presentation : **INOR.P-168**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Nickel-Catalyzed Anionic Cross-Coupling Reaction of Lithium Sulfonimidoyl Alkylidene Carbenoids With Organolithiums, followed by extensive DFT Methods.

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²*Organic Chemistry, RWTH Aachen University, Korea*

In the past 30 years, Professor Hans-Joachim Gais and his group have been in pursuit of pioneering a new catalytic reaction, a nickel(0)-catalyzed anionic cross-coupling reaction (ACCR) of lithium and magnesium sulfonimidoyl alkylidene carbenoids (metalloalkenyl sulfoximines) with organometallics, affording substituted alkenylmetals and sulfinamide. In the absence of a Ni(0)-catalyst or Ni(II)-pre-catalyst no ACCR occurs. Cleavage of the C-S bond occurs with complete retention of configuration at the S atom. Whilst a catalytic cycle was proposed for the Ni(0)-catalyzed ACCR of lithium sulfonimidoyl alkylidene carbenoids based on the formation of alkenyl Ni(0)-ate complexes, the mechanisms were deemed to archaic and moreover was vague; thereby we aimed to make adjustments to illustrate an up to date mechanism. In doing so, DFT methods were employed to buttress the experimental data presented and to devise a completely new catalytic cycle with respective appropriate mechanisms and energy profile diagrams. Notable features included the high stabilisation of the Li⁺-coordinating to either Ni, O, or N. Furthermore, we performed various extensive computational calculations in quest of finding an improved stereochemistry-yield by manipulating multiple factors including the solvent, conformations of the adduct and starting materials, and positioning the Ni(0) catalyst.

Poster Presentation : **INOR.P-169**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Photophysical study for *N,C*-chelate organoboron complexes including *o*-carborane cluster

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N,C-chelate organoboron complexes have attracted great attention in optoelectronic application such as organic light emitting diodes(OLEDs) and photovoltaic cells due to their high thermal stability and excellent photophysical property. In particular, various functional groups are introduced to four coordinate organoboron compounds for standing out their intrinsic properties. Among them, we have been interested in 1,2-*closo*-C₂B₁₀H₁₄ (*o*-carborane) as a substituent of organoboron complexes since it possesses unique chemical properties such as a highly polarizable σ -aromatic character and good thermal and electrochemical stability. In this study, we demonstrate the synthesis of *N,C*-chelate organoboron complexes including *o*-carborane cage and their intriguing photophysical characters.

Poster Presentation : **INOR.P-170**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

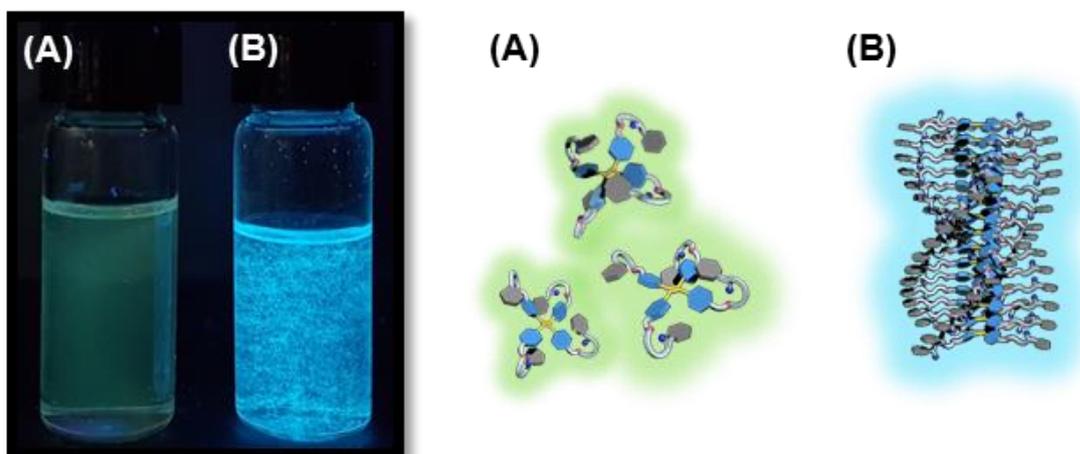
Mechanically Controlled Supramolecular Polymerization

Seonae Lee, Ka Young Kim¹, Jong Hwa Jung^{1,*}

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¹Department of Chemistry, Gyeongsang National University, Korea

We investigated the self-assembled behavior in THF with mechanical control. **TPE-2** building block was introduced with tetraphenylethylene (TPE) showing Aggregation Induced Emission effect and a chiral amide group for hydrogen bonding interaction. We analyzed the rate of polymerization using the characteristics of **TPE-2**. The self-assembled **TPE-2** showed the weak greenish emission without external stimuli. In contrast, the self-assembled **TPE-2** revealed the strong blue emission with stirring and sonication. The blue fluorescence intensity of **TPE-2** was dependent to the external stimuli such as stirring rate or sonication power. Furthermore, the positive CD signal of **TPE-2** enhanced gradually with external stimuli, indicates that **TPE-2** molecules were orientated to the left-handed helicity. Also AFM image of **TPE-2** building block showed M-helical aggregates. In this conference, we will present the self-assembled behavior of **TPE-2** in detail.



Poster Presentation : **INOR.P-171**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Mechanically reversible metal-organic gels based on titanium

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Titanium dioxide (TiO₂) is well known for photo-redox properties that facilitate its various applications such as photo-induced water splitting, CO₂ reduction, and chemical degradation. However, the surface modification of and the introduction of porosity into TiO₂ is quite difficult owing to their structural rigidity and robustness of TiO₂. Recently, many of the researches have been conducted to develop the new types of titanium-based materials such as Ti-oxo clusters and porous metal-organic frameworks (MOFs) to attain the efficient photocatalytic activities. In this study, we report novel titanium-organic gels exhibiting reversible sol to gel and gel to sol transformation and hierarchical porosity upon the removal of solvent molecules. The transparent, moldable, and injectable titanium-organic gels are obtained by heating the solution of titanium clusters and organic ligands. These gels readily become sols through a physical stimulus, shaking at low temperature. In addition, the porous titanium-organic aerogel was obtained through CO₂ supercritical point drying of the gels and was characterized by N₂ adsorption and desorption isotherm measurements. Even though the titanium clusters used as gelators of the titanium-organic gels have no porosity, the dried aerogels possess hierarchical micro-, meso-, and macropores. The prominent photochromic property was verified by UV irradiation and applied in light-induced dye degradation. This research suggests the versatile method to prepare stimuli-responsive and porous photocatalysts.

Poster Presentation : **INOR.P-172**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and characterization of zinc(II) coordination polymers with bis-1,4-(di-4-pyridylaminomethyl)benzene.

Ahrim Jeong, Kil Sik Min^{1,*}

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¹*Department of Chemistry Education, Kyungpook National University, Korea*

The design and assembly of transition metal-based coordination polymers have attracted much attention because of their potential applications in the areas of materials such as catalysis, magnetism, adsorption, and photoluminescence. Two new zinc(II) coordination polymer, $[(\text{dpab})\text{Zn}_2(\text{CH}_3\text{CO}_2)_2]_n$ (**1**) and $\{[(\text{dpab})\text{Zn}(\text{H}_2\text{O})_2](\text{NO}_3)_2\}_n$ (**2**) (dpab = bis-1,4-(di-4-pyridylaminomethyl)benzene), have been synthesized by the reaction of dpab ligand and $\text{Zn}(\text{CH}_3\text{CO}_2)_2 \cdot 2\text{H}_2\text{O}/\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$. Compounds **1** and **2** have been characterized by infrared spectroscopy, elemental analysis, X-ray structural analysis, and photoluminescence. In complex **1**, zinc(II) ion has a distorted tetrahedral geometry with two nitrogen atoms of the coordinated ligand and two oxygen atoms from acetate anions. In complex **2**, zinc(II) ion has a distorted tetrahedral geometry with two nitrogen atoms of the coordinated ligand and two oxygen atoms from water molecules. Compounds **1** and **2** were formed 2D polymers and show strong emission at 355 and 387 nm, respectively. In this poster, we will present the detailed preparation, crystal structure, and properties.

Poster Presentation : **INOR.P-173**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Effects of Metal Substitution in Topological Isomeric MOFs on Water Vapor Sorption

Nakyung Lee, Hyungphil Chun*

Department of Applied Chemistry, Hanyang University, Korea

Atmospheric water vapor sorption using porous materials has been studied toward a variety of practical applications such as fresh water harvest or dehumidification. MOFs are regarded as proper medium in this field because of potential voids which can be repeatedly filled and removed with guest molecules. ZBDt and ZBDh are topological isomeric MOFs composed of Zn, terephthalic acid, and 1,4-diazabicyclo[2.2.2]octane in a 2:2:1 ratio with square and hexagonal channels, respectively. These MOFs provide an ideal platform where the effects of pore structure on sorption characteristics can be studied. Therefore we studied the influence of various chemical and physical environments of pores on water vapor sorption by ZBDt/ZBDh homologues. Zn in the paddle wheel SBU was partially or completely substituted with Co, Cu, and Ni by room temperature and solvothermal reaction. The structures of homologues were confirmed by PXRD. The reversible water vapor sorptions were measured under both static and dynamic flow conditions. Their structural stabilities and water vapor sorption characteristics are compared.

Poster Presentation : **INOR.P-174**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Cytotoxic and Anticancer Properties of New Ruthenium Polypyridyl Complexes

Jinheung Kim^{*}, Tikum Florence Anjong¹, Fortibui Maxine Mambo²

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

²*Chemistry, Ewha Womans University, Korea*

The ligand exchange kinetics of metal complexes in aqueous solution, which are crucial for anticancer activity and vary for different metal ions, are very similar for platinum and ruthenium complexes. Their relatively low toxicity and ability to mimic iron in binding to biomolecules have made ruthenium complexes an attractive alternative to platinum-based drugs, since cancer cells overexpress transferrin receptors to satisfy their increased demand for iron. In this report, three ruthenium complexes containing a bidentate piq ligand, [(piq)Ru(bpy)₂]²⁺ (1), [(piq)Ru(phen)₂]²⁺ (2), and [(piq)Ru(DIP)₂]²⁺ (3) (piq = phenylisoquinolate, bpy = 2,2'-bipyridine, phen = 1,10-phenanthroline, DIP = 4,7-diphenyl-1,10-phenanthroline), were prepared. The DNA binding properties of complexes 1~3 to double-stranded DNA were studied. The binding of 1~3 to calf-thymus DNA yielded lower emission intensities than those observed with the corresponding Ru complexes alone. To explore potential interactions of complexes 1~3 with lipid-rich organs in live cells, the emission properties of the Ru probes were studied with liposomes. The emission intensities of complexes 1~3 were enhanced to similar extents upon interaction with liposomes. The cytotoxic activities of the complexes against MDA-MB-231 and HUVECs was evaluated in vitro. The effects of complexes 1~3 on the survival of MDA-MB-231 cells were examined and compared with that of cis-platin. Complexes 2 and 3 were more cytotoxic to cancer cells than cis-platin. Complexes 1~3 showed cellular uptakes of 1.1, 10.6, and 76.6 %, respectively, indicating that the greatest amount of complex 3 entered the cancer cells.

Poster Presentation : **INOR.P-175**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Electrocatalytic Hydrogen Production by New Cyclopentadienyl Rhodium Catalysts

Jinheung Kim

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

The production of hydrogen from water using solar light energy has attracted great interest for the production of a clean, sustainable fuel that may help address the current dependence on fossil fuels. The electrocatalytic activity of two new molecular rhodium catalysts was investigated in a hydrogen evolution system in the presence of a proton source using glassy carbon electrodes in acetonitrile and water. Rhodium complexes supported by pbi and pbt ligands, i.e., $[\text{Cp}^*\text{Rh}(\text{pbt})\text{Cl}](\text{PF}_6)$ (1) and $[\text{Cp}^*\text{Rh}(\text{pbi})\text{Cl}]$ (2) (where Cp^* is pentamethylcyclopentadienyl, pbt is 2-(2'-pyridyl)benzothiazole, and pbi is 2-(2'-pyridyl)benzimidazole), were observed to electrocatalytically evolve H_2 at potential of -0.90 V vs Ag/AgCl in CH_3CN and $\text{CH}_3\text{CN}/\text{H}_2\text{O}$. Cyclic voltammetry of 1 and 2 in the presence of acid revealed redox waves consistent with the Rh(III)/Rh(I) couple. Bulk electrolysis were used to confirm the catalytic nature of the process for complexes 1 and 2, with turnover numbers in excess of 100 and essentially quantitative faradaic yields for H_2 production. The potentials at which these Rh complexes catalyzed H_2 evolution were close to the thermodynamic potentials for the production of H_2 from protons in CH_3CN and $\text{CH}_3\text{CN}/\text{H}_2\text{O}$, with the small overpotential being 50 mV for 1 as determined by electrochemistry. The complex 1 with more positive Rh(III/I) redox potentials exhibited higher activity for H_2 production.

Poster Presentation : **INOR.P-176**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Application of immunosensor using QD Immobilized Silica Nanoparticles for signal amplification

Daekyung Sung

*Center for Convergence Bioceramic Materials, Korea Institute of Ceramic Engineering and Technology,
Korea*

QD functionalized silica nanoparticles was developed for application of immunosensor using nonbiofouling, pre-activated polymers coated substrates for cancer marker detection. In this work, we synthesized random copolymers having three important groups: anchoring sites, serving to attach the COC substrate; a PEG component, which acts as a repellent of non-specific biomolecules; and an NHS ester group for conjugation of biomolecules. For sandwich immunoassays, anti- α -fetoprotein (Anti-AFP) as capture antibody was covalently immobilized on the substrate through the polymer layers. Furthermore, we prepared anti-AFP/QD-coated silica nanospheres conjugates for signal amplification. Sandwich-type immunoassays were carried out on the polymer coated COC surfaces using AFP (liver cancer marker). Using the optimized assay, the red fluorescence response to AFP was linear over a range from 0.1 to 100 ng/ml.

Poster Presentation : **INOR.P-177**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of a RGB Narrow-Bandwidth Stop Filter by Simulating and Depositing Nano-Multi-layers

**Gang Yeol Yoo, Young Kwon Jang¹, JoongHo Lee¹, Byungju Lee¹, Woong Kim^{2,*}, Young
rag Do^{3,*}**

Department of Advanced Materials Engineering, Korea University, Korea

¹*Chemistry, Kookmin University, Korea*

²*Division of Advanced Materials Engineering, Korea University, Korea*

³*Department of Bionano Chemistry, Kookmin University, Korea*

Narrow-bandwidth stop filters (NBSF) with red, green, and blue (RGB) colors were fabricated by depositing materials with a low refractive index and a high refractive index in an alternating approach. These RGB NBSFs, fabricated by periodically depositing SiO₂ and Al₂O₃, were simulated using an “OpenFilters” simulation. Though it is not easy exactly to determine the simulated data of the NBSF due to the complex changes in several related parameters, certain parameters are critical for determining simulated data, such as the thickness, refractive index and the stacking pairs. The full width at half maximum (FWHM) of the reflectance of the RGB NBSF was approximately 50 nm, and the reflectance of the RGB NBSF exceeded 90 %. The optical properties of the RGB NBSF were examined by means of reflectance and transmittance spectroscopy. The structural properties of the RGB NBSF were studied using a transmission electron microscope measurement by preparing focused ion beam (FIB) in slice mode.

Poster Presentation : **INOR.P-178**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhancement of the Thermal Stability of InP/ZnSeS/ZnS Quantum Dots by a Polysilazane (PSZ) Coating Process

Hyeongjin Lee, Hee Chang Yoon¹, Young rag Do^{2,*}

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We synthesized InP/ZnSeS/ZnS quantum dots (QDs) and coated polysilazane (PSZ) onto the synthesized QDs. The coated QDs were more stable than pristine QDs. Si-N-based PSZ can cover the surfaces of the ligands of QDs to form an inorganic encapsulant. Therefore, the PSZ coating layer can prevent the detachment of ligands after a thermal treatment. The photoluminescent quantum yield (PLQY) of pristine QDs decreased by 52.0%, whereas the PLQY of the PSZ-coated QDs increased by 44.6% after thermal treatment (150 °C, three days). It can be considered that the ligand detachment from InP QDs is induced by thermal damage and by the degradation of optical properties such as the PLQY and the full width at half maximum (FWHM). We will discuss the change of optical and chemical properties of both pristine and PSZ-coated InP QDs as functions of thermal and moisture damages.

Poster Presentation : **INOR.P-179**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of Free-Standing Quantum Dot Films for Remote-type White LEDs

Soyeon Yoon, Hee Chang Yoon, Yun Jae Eo, Keyong Lee¹, Young rag Do^{2,*}

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This study introduces free-standing quantum dot (QD) films using AgIn₅S₈/ZnS (AIS) QDs as a down-conversion (DC) material for the remote-type white light-emitting diodes (WLEDs). The QDs are not suitable for use in in-cup types of WLEDs as a DC material due to direct heat. Therefore, we introduce remote-type WLEDs which involve simply putting the free-standing QD films on a blue LED to reduce the thermal damage of QDs. We synthesized the AIS QDs using a hot injection method. The AIS QDs showed a dominant wavelength of 530 nm, a broad band-width of 95 nm and a photoluminescent quantum yield (PLQY) of 64%. Next, we fabricated free-standing QD films using an electro-spray (e-spray) method. The AIS QDs and poly(methylmethacrylate) (PMMA), were used as a DC material and a matrix, respectively. To realize the WLEDs, the free-standing QD films were simply placed on an InGaN blue LED. The WLEDs show correlated color temperature (CCT, K) of 5500, 4100 and 3800 K and luminous efficacy (LE) of 76, 69 and 65 lm/W with 3, 4.5 and 6 hours e-sprayed free-standing QD films, respectively, at an applied current of 60 mA. The color rendering index (CRI, Ra) of the WLEDs were 71, 61 and 59 with the 3, 4.5 and 6 hours e-sprayed free-standing QD films, respectively. The low CRI is due to lack of reddish color, though this can be improved by using red QDs mixed with green QDs. These results demonstrate the possibilities of QD films for WLEDs.

Poster Presentation : **INOR.P-180**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication and Characterization of Green & Red CsPbX₃/CsPb₂Br₅ Perovskite Quantum Dot Films

Hee Chang Yoon, Hyeongjin Lee, Heejoon Kang, Young rag Do^{1,*}

Department of Chemistry, Kookmin University, Korea

¹*Department of Bionano Chemistry, Kookmin University, Korea*

We synthesize highly efficient and stable green CsPbBr₃/CsPb₃Br₅ and red CsPb(Br_{0.35}I_{0.65})₃/CsPb₂Br₅ core/shell perovskite quantum dots (PeQDs) which are capable of realizing high color purity and a wide color gamut. The synthesis process is conducted by means of facile colloidal hot injection with more precursor and longer reaction times compared to those of the CsPbX₃ reaction method. The quantum yields of the green and red core/shell PeQDs were increased by nearly 10% compared to those of core PeQDs. In addition, to fabricate the core/shell PeQD films, we introduced a polyurethane-based polymer binder. The optical properties of the synthesized CsPbX₃/CsPb₂Br₅ quantum dots were measured according to the photoluminescence and electroluminescence, and the structural properties were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM).

Poster Presentation : **INOR.P-181**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Selective sensing of nitroaromatic compounds using fluorescent MOF

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

Drastic use of explosive type of materials in terrorism activities all around the world made it highly desirable to detect the traces of explosives materials with the easy and cost effective manner for security, military issues and environmental protection. Trinitrophenol (TNP) has the higher explosive power amongst the nitro aromatic explosives even more than trinitrotoluene (TNT) and causes strong irritation and allergic reactions.¹ Plenty of works are reported using MOFs to selectively sense TNP featuring Lewis basic pyridyl or free amine sites inside the pores that are expected to induce electrostatic and hydrogen-bonding interactions. However, no direct evidence has been affirmed till date about the interaction of TNP molecule with MOF which leaves the sensing mechanism of TNP and the use of other functionality in ambiguity. We synthesized new MIL-53 analogous MOF using Indium nitrate which shows high water stability and strong fluorescence. We predicted that availability of hydroxyl group would provide hydrogen bonding and pi-pi interaction with TNP molecule and align it in the close proximity to the host functionality for the plausible electron transfer and resonance transfer mechanism enhancing fluorescence quenching. The MOF was used for sensing of Nitro aromatic compounds (NAC) which are considered highly explosive and toxic and shows very high selective quenching for TNP.² We further investigated the dynamic of quenching, performing fluorescence lifetime experiment which resulted in no change for fluorescence lifetime of MOF and suggests that static quenching is the major reason behind quenching of TNP. Spectral overlap of absorbance of analytes and the emission of MOF indicate highest possibility of energy transfer mechanism for TNP in as compared to others.

Poster Presentation : **INOR.P-182**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Biomolecular Logic Computation using Nanoparticles on Lipid Bilayer

Sungi Kim, Jwa-Min Nam*

Division of Chemistry, Seoul National University, Korea

Computation is a ubiquitous concept/method in physical sciences, biology, and engineering that provide controllability, programmability and processibility. There has been an ongoing effort to merge computation with “unusual” matters across many length scales, from microscopic droplets to DNA nanostructures and molecules. However, the implementation of complex computation in particle systems, especially in nanoparticles, remains particularly challenging, despite a wide range of potential applications that would benefit from controlling their unique optical, optoelectronic, plasmonic, magnetic, catalytic, structural, and other material properties at the nanoscale, without human interventions. This is mostly due to the lack of scalable architectures that enable systematic integration and wiring of the gates into a large integrated circuit on a reliably analyzable platform. Further, DNA/RNA computing has been highly promising due to nearly unlimited programmability, high-density information storage and application potentials in biomedical systems, but its practical applications are largely limited due to lack of spatial isolation, non-reusable gates, and poor scalability and analyzability. Here we report the development of a nanoparticle-lipid hybrid-based computing platform termed lipid nanotablet (LNT), in which nanoparticles, each programmed with surface chemical ligands, are tethered to a supported lipid bilayer chip to carry out computation. Supported lipid bilayers, which have been used as synthetic mimics for cell surfaces, are used here as chemical circuit boards for nanoparticle circuits. DNA sequences are used as molecular inputs to induce change in plasmonic coupling signals based on assembly and disassembly between DNA-modified metal nanoparticles.

Poster Presentation : **INOR.P-183**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Channel opening of columnar coordination network for detection of polycyclic aromatic hydrocarbons

Jaejun Kim, Masaki Kawano*

Department of Chemistry, Tokyo Institute of Technology, Japan, Japan

In principle, porous coordination networks (PCNs) which have been in the limelight as porous materials for various kinds of application are considered to enable to produce the designable structure by controlling the metal nodes and bridge ligands. However, their self-assembly nature gives rise to various kinds of geometry that sometimes we do not intend. Post-synthesis modification can be a strong strategy to produce designable structure for target application. Herein, we report the intercalated channel opening of highly packing structure by simple post-synthetic removing of mono-dentate ligand layer selectively and its absorption ability for polycyclic aromatic hydrocarbons.

Poster Presentation : **INOR.P-184**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

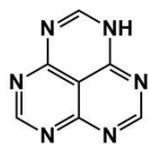
Multi-carboxylic acids as co-ligands to extend voids in the structure of zinc and TPHAP coordination system

Krittanun DEEKAMWONG, Hiroyoshi OHTSU, Masaki KAWANO*

chemistry, Tokyo Institute of Technology, Japan

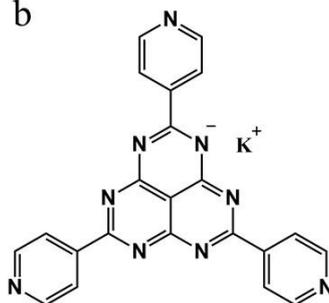
Porous coordination networks (PCNs) are designable materials by controlling an organic linker or a metal precursor. PCNs have been intensively studied for potential applications such as molecular sieve, catalysis, and sensor. We designed multi-interactive pyridyl ligands having a hexaazaphenalene (HAP) skeleton. We selectively generated various kinds of coordination networks using HAP ligands and Ni^{II}, Cu^{II}, Cu^I, Co^{II}, Cd^{II}, especially Zn^{II} metal ions by thermodynamic/kinetic control.[1] Here, we report the solvothermal syntheses of PCNs using zinc ions, TPHAP, and dicarboxylic acids as co-ligands. A DMF solution of K⁺TPHAP⁻, co-ligands and a zinc ion were heated at 90 degree C for 24 h. A structure of the crystalline product was determined by single crystal X-ray diffraction analysis. In this presentation we will discuss the structural and electronic properties of networks and utilize their expanded void spaces.

a



HAP

b



K⁺TPHAP⁻

c



Poster Presentation : **INOR.P-185**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Control of Cellular Behavior on Nanostructured Surface by Chemical Effect

YunYeong Lee, Jin seok Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Cellular interactions with complex extracellular matrix (ECM) play a crucial role in the control of cellular behaviors, such as cell adhesion, migration, proliferation, and differentiation, which are related with mechanotransduction signaling pathway, however, how cell adhesion on the surface nanotopographies affects the cellular behaviors have not well known, due to complex focal adhesion dynamics. Also, one of the various factors that affect the cellular behaviors is 'chemicals'. However, many of the substances that promote or inhibit the various actions of cells are known, but there is insufficient study of the cellular behaviors that occurs when they work with the effects of surface. Here we explored the cellular behaviors after treating chemicals on various surfaces nanotopography of silica beads to promote or inhibit the cell adhesion.

Poster Presentation : **INOR.P-186**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of Various Dimensional Embossed Substrates with Expander

Yoobeen Lee, Jin seok Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Micro- and Nanostructures are important to use as a building blocks in modern science and technology. Especially, there are many researches for preparation of embossed surfaces using beads like silica or polystyrene with a variety of sizes. However, research on fabrication of substrate with different distance between beads has not been studied yet. So, we easily manufactured substrates whose embossed parts expanded with same interval using hand-made device, 'Expander' and PDMS. In this work, we figured out some optimized conditions for making PDMS such as hardening time for imprinting, thickness and ratio of base to agent for expanding well. Each elasticity of PDMS is measured with tensile strength meter. We prepared PDMS templates with random, hexa- and cubic-array, and assembled various sized silica beads. And then, we expanded the PDMS variously and transferred them to 1*1 cm² glass substrate immediately. Finally, we fabricated the various dimensional embossed substrates.

Poster Presentation : **INOR.P-187**

Inorganic Chemistry

Grand Ballroom, FRI 11:00~12:30

Heterometallic BODIPY-Based Molecular Squares obtained by Self-assembly: Synthesis and Biological Activities

Yeji You, Gajendra Gupta¹, Chang Yeon Lee^{1,*}, Dong-Ku Kang^{*}

Department of Chemistry, Incheon National University, Korea

¹*Department of Energy and Chemical Engineering, Incheon National University, Korea*

Metal-based multinuclear supramolecules of different functionality designed by self-assembly process has been a growing area of research due to their versatile applications. Four new bodipy based octacationic heterometallic molecular squares 3-6 were synthesized by self-assembly process by reaction of dipyrityl bodipy ligands with suitable 90° palladium and platinum acceptors. The formation of the as-synthesized molecular squares were confirmed by different analytical techniques using multinuclear NMR spectroscopy, elemental analysis, high resolution electrospray mass spectrometry (HR-ESMS), UV/Vis and PL spectroscopy. The cytotoxicity of the new supramolecules and the starting precursors were studied against colorectal carcinoma (HCT116), prostate adenocarcinoma (PC-3), breast adenocarcinoma (MCF-7), lung adenocarcinoma (A549) and non-malignant human kidney epithelial (HEK-293) cell lines using MTT assay. To determine the intracellular localization of supramolecules, their auto-fluorescence was a good tool for searching supramolecules. The cell death action mechanism of supramolecules was identified with two cell lines that had good cytotoxicity activity were stained with FITC conjugated Annexin-V and propidium iodide (PI).

Poster Presentation : **INOR.P-188**

Inorganic Chemistry

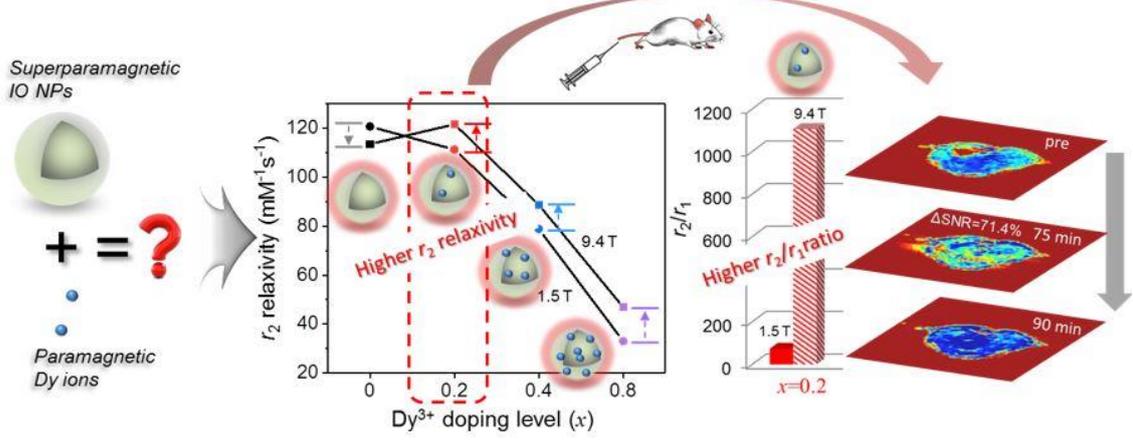
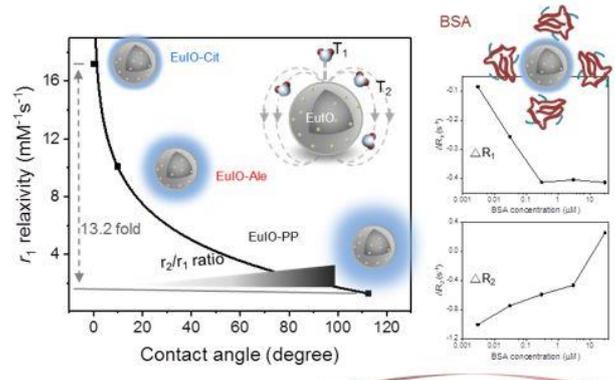
Grand Ballroom, FRI 11:00~12:30

Lanthanide-engineered iron oxide nanoparticles: surface design-dependent magnetic relaxivity tuning and high-performance T2 MRI nanoprobes in ultrahigh magnetic field

Jeong Chan Park

Pohang University of Science and Technology, Korea

Magnetic nanoparticles (NPs) engineered by doping with lanthanide (LN) have attracted considerable attention due to their unique optical and magnetic properties. However, to date, the studies have focused on synthesis and the development of T1-T2 dual-modal MRI contrast agents (CAs) utilizing lanthanide ions. Here, we show that Gd-engineered ultras-small magnetite NPs do undergo the Verwey transition at ~ 110 K and that surface anisotropy is an important factor in such a transition. In addition, we report the relaxivity tuning of T1-T2 dual-modal MRI nanoprobes (DMNP) depending on the surface design, and the monitoring protein interactions with DMNP. To date, the realization and the relaxivity tuning of DMNP have been attained through the dopant, size and morphology of nanomaterials, remaining open opportunities for sensing applications of DMNP. We observe that the correlation between the hydrophobicity of surface materials and the longitudinal relaxivity (r_1) of DMNP presents exponential decay feature. According to the surface materials of DMNP, DMNP can act as T1-T2 dual-modal or T2-dominant MRI CAs. It is also explored that the feasibility of the resulting nanosystem as a biosensor to report environmental changes, such as albumin interaction. The albumin interaction on DMNP shows the change in both T1 and T2 relaxation time, which would be the mutually confirmative information. Dy-engineered iron oxide nanoparticles show the high performance contrast ability at ultrahigh magnetic field (9.4 T) compared with the reported one. Detailed experiment methods and results would be presented at this meeting.



Poster Presentation : **PHYS.P-189**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Folding Free Energy Landscape of Ordered versus Disordered Proteins

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The funneled landscape perspective has served as a conceptual background for understanding protein folding, but the explicit characterization of the protein free energy landscape from fully microscopic approaches remains a challenge. Here, we propose a simple and direct construction method of the landscape based on all-atom simulations. We apply it to representative alpha-helical (HP-35) and beta-sheet (WW domain) proteins and to an intrinsically disordered protein (pKID) that folds upon binding to its partner (KIX) to extract common and distinctive characteristics of their landscapes. We find that pKID, as well as HP-35 and WW domain, possesses the funneled landscape, but its landscape is not funneled enough to allow the folding by itself; nevertheless, the landscape of pKID becomes funneled enough upon binding to KIX. The method proposed here is applicable to any atomistic simulations, and will be effective in deriving molecular insights behind a variety of biomolecular processes.

Poster Presentation : **PHYS.P-190**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Nucleophilic Substitution Reaction of Anthraquinone-2-Carbonyl Chloride

Han joong Koh

General Science Education, Jeonju National University of Education, Korea

The nucleophilic substitution reaction of anthraquinone-2-carbonyl chloride (1) were studied kinetically in various mixed solvents. The analysis using the extended Grunwald-Winstein equation in the reaction of anthraquinone-2-carbonyl chloride obtained the ρ value of 2.11, the m value of 0.54, and the correlation coefficient of 0.955. The nucleophilic substitution reaction of 1 might proceed via an associative S_N2 mechanism enhancing bond making than bond breaking in the transition state..

Poster Presentation : **PHYS.P-191**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Molecular Design of Porphyrin-Based Sensitizers for Use in Dye-Sensitized Solar Cells

Liezel Estrella, Sang Hee Lee, Dong Hee Kim*

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Considerable and extensive research efforts have been dedicated to design and synthesis novel dyes with the goal of improving the efficiency of DSSCs for almost three decades. The progressive development of computational chemistry has paved way for chemists to conduct realistic study on the structure-property relationship of the molecules through running computer simulations. This study aims to engineer a high-performing porphyrin-based sensitizers based on SM315 dye. DFT and TD-DFT methods were used to conduct a computational study of dye-to-semiconductor interaction and charge transfer mechanism of novel porphyrin-based dyes by calculating the geometry, photophysical and electrochemical properties of the dyes and the dye-TiO₂ complexes. This theoretical research provides profound understanding concerning the dye-to-semiconductor electronic interaction and charge-transfer mechanism in dye-sensitized solar cells.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Interactions of naphthol-based photoacids with bovine and human serum albumins investigated by the excited-state proton transfer reaction

Seong-June Lee, Han Gook Cho*, Byeong-Seo Cheong*

Department of Chemistry, Incheon National University, Korea

The interactions of several different naphthol-based photoacids with bovine and human serum albumins have been investigated by observing the excited-state proton transfer (ESPT) of photoacids. Two bands due to the protonated and deprotonated forms of the photoacid were observed in the fluorescence emission spectra, and the fluorescence intensity ratios of the two bands were monitored as the concentration of bovine or human serum albumin in phosphate buffer was varied. It was found that the variation of the fluorescence intensity ratios of the two forms, and thus the degree of the ESPT process, was significantly different depending on the position of the hydroxyl and sulfonate groups of the photoacid as well as the type of serum albumin. The possible binding interaction and configuration of the photoacid in the binding site of serum albumin were discussed.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Excited-state proton transfer of 2-naphthol-6,8-disulfonate in various reverse micelle environments

Su-Hyun Kang, Han Gook Cho*, Byeong-Seo Cheong*

Department of Chemistry, Incheon National University, Korea

The excited-state proton transfer (ESPT) reaction of 2-naphthol-6,8-disulfonate, a photoacid dye, has been studied in several different reverse micellar solutions formed from various cationic, anionic, and nonionic surfactants. Fluorescence emission was observed from the protonated and deprotonated forms of 2-naphthol-6,8-disulfonate, and the degree of ESPT reaction in the reverse micelle was estimated by observing the fluorescence emission intensity ratio of the two bands. The reverse micelles contain a small water environment, with the amount of water usually denoted by the W_0 value. The fluorescence intensity ratios were measured as a function of the W_0 for each reverse micelle studied, and the effects of adding long-chain alcohols as a co-surfactant or adding salts were also investigated. The observed behaviors were discussed in terms of interactions of the dye in the water pool.

Poster Presentation : **PHYS.P-194**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Varying anisotropy in thermal oxidation of two-dimensional transition metal dichalcogenides

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

In-plane anisotropy in various material properties of two-dimensional (2D) crystals is not only intriguing but also of potential use for many applications. In this work, we studied how the structural anisotropy influence oxidation of 2D semiconducting transition metal dichalcogenides (TMDs) in the form of MX_2 , where $\text{M} = \text{Mo}$ and W ; $\text{X} = \text{S}$ and Se . Single and few-layer TMD samples mechanically exfoliated on SiO_2/Si substrates were characterized for thickness by their differential reflectance and thermally oxidized in controlled $\text{Ar}:\text{O}_2$ mixture at elevated temperatures of $280 \sim 380$ °C. Oxidation was initiated from randomly distributed reaction centers and led to triangular oxides (TOs) and triangular etch pits (TEs) that were revealed by atomic force microscopy (AFM) measurements. The TOs and TEs in WX_2 were more rounded than those in MoX_2 indicating more anisotropic reactions occur in the latter. In addition, the density of TOs and TEs was 30 times higher in MSe_2 than MS_2 , which suggests that MSe_2 contains more reaction centers, possibly structural defects. Finally, MoSe_2 and WS_2 showed the lowest and highest reaction barriers, respectively, which will also be discussed with the observation that only WS_2 did not exhibit etch pits.

Poster Presentation : **PHYS.P-195**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Twist-angle dependent optical second-harmonic generation from MoS₂/WS₂ heterostructure

Wontaek Kim, Sunmin Ryu*

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

Optical second-harmonic generation (SHG) by single and few-layer transition metal dichalcogenides (TMD) is highly efficient and sensitive to their structural symmetry. Recently, it was reported that the SHG signal from artificially-stacked MoS₂ (molybdenum disulfide) bilayers can be understood as superposition of SHG fields from the individual layers. However, it has not been verified whether this model is still valid for TMD heterostructures. In this work, we studied SHG behavior of artificially-stacked MoS₂/WS₂ (tungsten disulfide) hetero-bilayers of varying twist angle in comparison with MoS₂ homo-bilayers. Polarization-resolved SHG polar plots from MoS₂ homo-bilayers exhibited a six-petal pattern like those from MoS₂ monolayer. Remarkably, we found that polarization-resolved SHG behavior of MoS₂/WS₂ is much different from that of MoS₂ bilayers. Unlike the homo-bilayers, the hetero-bilayers exhibited constant background signal in addition to the six-petal pattern. This anomalous background became bigger for more staggered hetero-bilayers. To explain these results, we propose that the anomaly originates from SHG phase difference between MoS₂ and WS₂, and will corroborate its validity with phase-resolved SHG measurements and numerical simulations.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Difference between results of random walk simulations and diffusion-reaction theory in two and three dimensions

Junmyeong Jeong, Taehyun Yun¹, Taejun Kim*, Hyojoon Kim*

Department of Chemistry, Dong-A University, Korea

¹*Dong-A University, Korea*

The random walk simulation usually predicts the theoretical results in the diffusion-influenced reaction field with accuracy in various dimensions. While one dimensional results of simulation and theoretical approaches are in agreement, significant differences are shown between simulation and theoretical results in two and three dimensions. We have quantified the difference rigorously. We study why the differences exist in higher dimensional results and suggest the optimum lattice constants.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Interactions between water-soluble polymer and surfactant molecules studied by the excited-state proton transfer of pyranine

Hyomin Kim, Han Gook Cho^{*}, Byeong-Seo Cheong^{*}

Department of Chemistry, Incheon National University, Korea

The interactions of cationic surfactants, alkyltrimethylammonium bromide, with polymers in aqueous solutions have been studied by utilizing the excited-state proton transfer (ESPT) of pyranine (8-hydroxypyrene-1,3,6-trisulfonate) as a probe. The water-soluble polymers such as poly(vinyl alcohol), polyvinylpyrrolidone, and poly(acrylic acid) were used in the study. Fluorescence emission was observed from the protonated and deprotonated forms of pyranine. As the concentration of either a polymer or a surfactant varied in aqueous surfactant/polymer solutions, there were considerable changes in the fluorescence intensity ratios of the two bands and in the maximum emission wavelengths. These were related with the change in the critical association concentration of micelles, and the possible interactions between the surfactant and polymer were discussed. In addition, the effects of changing the chain length and molecular weight of the polymer were investigated.

Poster Presentation : **PHYS.P-198**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Surface-enhanced Raman spectroscopy and density functional theory on riboflavin and related molecules adsorbed on colloidal silver particles

Minju Yun, Han Gook Cho^{1,*}, Byeong-Seo Cheong^{1,*}

Department of Chemistry, Incheon National University, Korea

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

A combined surface-enhanced Raman spectroscopy (SERS) and density functional theory (DFT) study on riboflavin and related molecules adsorbed on colloidal silver particles has been conducted to investigate the spectral vibrations among flavin compounds and the adsorption geometry on the metal surface. The SERS spectra were measured at different pHs to gain information on the adsorption geometry as well as the pH-dependent spectral variation. The Raman spectra of the compounds in powder form were also obtained for comparison with the SERS spectra. DFT calculations were performed to assign the vibration modes of observed bands and to model the adsorption geometry of riboflavin on the silver surface. The interactions of adsorbates with metal nanoparticles and the adsorbate conformation were discussed based on the observed spectra and DFT results.

Poster Presentation : **PHYS.P-199**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Formation and Photophysical Behavior of Two-Dimensional PTCDA Film (perylene-3,4,9,10-tetracarboxylic dianhydride) on Graphene

Dogyong Kim, Sunmin Ryu*

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

Two-dimensional van der Waals (2D vdW) heterostructures have recently gained much research interest due to their unusual properties and new phenomena. Despite their potential both in fundamental research and application, organic-inorganic 2D vdW heterostructures have not been under systematic spectroscopic investigation. In this work, PTCDA/graphene heterostructures were generated by self-limited assembly of organic vapors at elevated temperatures. Topographic details and photophysical properties of the heterostructures were studied by atomic force microscopy, micro-Raman, photoluminescence (PL) and reflectance spectroscopy. PL spectra exhibited significant progression with increasing thickness of PTCDA and their intensity was greatly quenched on metallic graphene. The quenching of strong PL signals revealed vibrational Raman features of PTCDA clearly on graphene. Absorption peaks identified from the reflectance measurements were attributed to molecular S_0 - S_1 transition, charge-transfer exciton and an unknown origin. The topographic and spectroscopic features will be discussed regarding their dependence on the thickness of PTCDA and graphene substrates.

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Raman Spectroscopic Study of Electronic Interactions between Graphene and Copper Substrates

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Raman spectroscopy has been a versatile tool to characterize various material properties of graphene such as structural defects, thickness, stacking, strain and charge density. While chemical vapor deposition (CVD) of graphene on copper substrates is one of the primary preparation methods for both fundamental research and industrial application, Raman scattering of as-grown graphene/Cu system has not been studied regarding how their interactions affect the electronic structure of graphene and thus its Raman spectra. In this work, we investigated as-grown graphene on Cu foils and Cu thin film/SiO₂/Si substrates using multi-wavelength Raman spectroscopy and atomic force microscopy (AFM). Excitation energy was varied in the range of 1.58 ~ 3.81 eV to minimize spectral interference of photoluminescence from Cu substrates. Most of all, both samples exhibited significant frequency deviations for G and 2D peaks with respect to those of freestanding reference samples. The smaller frequency changes observed for the latter samples were partly attributed to the less thermal expansion and compression of the substrates during the CVD growth. Secondly, 2D peak frequency of both samples were ~20 cm⁻¹ higher than expected even when the effects of strain and charge density were considered. Based on quantification of the effects of strain and charge density, we concluded that the unknown contribution was made by reduction in the Fermi velocity of graphene that was induced by its intimate interaction with underlying Cu substrates. The quantitative analysis of the change in the electronic structure given in this study will be highly useful in characterizing as-grown graphene and possibly in other forms.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Formation of Two-Dimensional Tetracene Crystals and their Photoluminescence Behavior on Graphene Substrates

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

Wave function and binding energy of an exciton are largely affected by not only its dielectric but also geometric environments. Excitons may be further confined in two-dimensional (2D) molecular crystals because of reduced dielectric screening. However, it has been a challenge to realize such molecular systems in a reproducible and spectroscopy-compatible manner. In this study, we created 2D tetracene films sandwiched between two graphene or hexagonal boron nitride (hBN) layers with high chemical stability and mechanical strength. To form such a vertical heterostructure, a top graphene (hBN) layer was dry-transferred onto tetracene film thermally evaporated on a bottom graphene (hBN) layer. Besides being a confining wall, graphene and hBN also served as an ideal 'spectroscopic window' due to their high optical transparency. Tetracene formed flat films with multiples of its minimum molecular layer and were found stable in the ambient conditions and even under intense laser irradiation. PL intensity substantially decreased when supported on graphene compared to on hBN, which indicates efficient energy transfer between tetracene and metallic materials. Efficiency of the PL quenching was also investigated as a function of number of graphene layers by steady-state emission measurements. Polarization-resolved PL analysis revealed a long-range order suggesting crystalline nature of 2D tetracene. We will discuss structural details and excitonic dynamics that will be probed by time-resolved spectroscopy. The demonstrated method will be highly useful in investigating the behavior of confined molecules and interactions between molecules and 2D materials.

Poster Presentation : **PHYS.P-202**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Comparative Nucleophilic Substitution at Carbon, Sulfur and Phosphorus Centers: ($S_N2@C$), ($S_N2@S$) and ($S_N2@P$)

Adhikary Keshab Kumar, Nasir Shahzad, Chan Kyung Kim*

Department of Chemistry & Chemical Engineering, Inha University, Korea

Three prototypical model systems for bimolecular nucleophilic substitution at carbon ($S_N2@C$), sulfur ($S_N2@S$) and phosphorus $S_N2@P$ were studied for finding the general phenomena using the B3LYP/6-311+G(d,p) level of theory. The models are chosen as:

At carbon, $X^- + CH_3C(=O)Y$ ($S_N2@C$)

At sulfur, $X^- + (CH_3)S(=O)_2Y$ ($S_N2@S$)

At phosphorus, $X^- + (CH_3)_2P(=O)Y$ ($S_N2@P$)

The $S_N2@C$ involves the characteristic transition state $[X-C(O)-Y]^-$ reflected in the double-well potential energy surface (PES). Similarly, it was found to be the same in the $S_N2@S$ system except for the asymmetric nucleophilic attack. We considered symmetric and asymmetric nucleophilic reactions in our model systems. In the case of symmetric nucleophilic attack at the phosphorus ($S_N2@P$), the reaction mechanism shows the double-well PES involving a transition state. In the case of asymmetric nucleophilic attack, two competing mechanisms were found: frontal or rear-side attack and the reaction mechanism depended on the conformation of the reactants.

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of Palladium Nanoparticles Deposited on CdS Nanorods by Pulsed Laser Ablation in Liquid: Effect of Size of Metal Nanocrystal in the Photocatalytic Hydrogen Production

Yujin Kim, Amaranatha Reddy, TaeKyu Kim*

Department of Chemistry, Pusan National University, Korea

Recently, photocatalysts comprising active sunlight-harvesting photo-absorbers and stable metal co-catalysts have attracted significant attention. However, the size, clean surface, and highly dispersed nature of the metal co-catalysts are crucial factors to affect catalytic performance and reaction rate. Nevertheless, most of the available metal nanocrystals have been synthesized by complicated procedures using harmful organic templates and stabilizers with difficulty and high cost. To overcome these problems, in this study, the pulsed laser ablation in liquid approach was applied to generate palladium and bimetallic palladium–platinum nanoparticles with an average size and distribution by adjusting the laser wavelength and fluence. They showed significantly improved amount of hydrogen evolution than that obtained by using bare CdS nanorods and several other noble-metal co-catalysts deposited on CdS . This proposed strategy is thought to open new avenues for the design of advanced photocatalytic materials for efficient solar-driven production of hydrogen.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dual Transition metal doped MoS₂ as an effocacious charge separator on CdS – Intensely active and stable visible light sensitive semiconductor for water splitting into hydrogen

Sumin Seo, Seunghye Kim, Praveen Kumar Dharani, Putta Rangappa, TaeKyu Kim*

Department of Chemistry, Pusan National University, Korea

The importance of hydrogen (H₂) played a major role as an substitute clean fuel to compete future energy demands. Therefore, its great demand to look for cost effective, highly efficient and renewable ways to produce hydrogen. Photo catalysis is considered an effective way to satisfy above challenges with no environmental issues. However, development of highly efficient photo catalysts which can function under visible light is still challenging. Herein, we report dual metal Fe-Co doped MoS₂ coupled onto one dimensional CdS nanorods to approach these. The photo catalytic performances of as prepared few layered Fe-Co doped MoS₂ integrated on to CdS (FCM/CdS) assessed by photo splitting of water into hydrogen in existence of lactic acid as a hole (h⁺) scavenger. The extraordinary hydrogen generation rate of 190 mmol·h⁻¹·g⁻¹ a 50 folds higher than that of bare CdS has been achieved. This improved activity arises from synergistic effects of dual transition metal doped MoS₂. Which promotes effective charge separation of photo generated carriers and improves the surface shuttling properties and enhanced hydrogen generation rate. The remarkable photocatalytic activity of FCM/CdS nanocomposites resulted from improved edge sites, enhanced electronic conductivity, and the existence of new active sites. The H₂ production rate achieved with bi-metallic doped MoS₂-based CdS photo catalyst for photo splitting of water is the highest activity observed to date. As a result, because of low cost and high efficiency of this system, it opens new windows for possible applications to use as a photo catalyst in various fields.

Poster Presentation : **PHYS.P-205**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Photodissociation Dynamics of Diiododifluoromethane in Solution

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To elucidate solvent role in chemical reaction in solution, complete photodissociation dynamics of CF₂I₂ in solution were obtained by probing C-F stretching mode after photolysis of these molecules with a UV photon. As in the gas phase, a state-selective photodissociation dynamics of CF₂I₂ was observed. 267 nm excitation leads to exclusive three-body decay and 350 nm to exclusive two-body decay. The generated CF₂ bimolecularly binds to produce C₂F₄ with a diffusion-limited rate. When excited at 267 nm, dissociated I atoms from 35 ~ 40% of a reacting molecule escape the solvent cage efficiently, CF₂I is produced by geminate rebinding (GR) of the interacting I atom and CF₂. All the produced CF₂I geminately rebinds with the remaining I atom and 64 ~ 80% of the dissociated CF₂ produces C₂F₄. When excited at 350 nm, CF₂ is produced via I₂-CF₂ isomer with a time constant of 14 ps ~ 48 ps that is rapidly formed from CF₂I and the dissociated I atom with a time constant of 0.5 ps. About 50% of CF₂I radical does not form the isomer and geminately rebinds with I atom with picosecond and nanosecond time scale. Thus, nascent photoproduct after 350-nm excitation, CF₂I takes three different reaction paths: isomer formation, fast and slow GRs. The subsequent reaction path of the nascent photoproduct is dictated by its internal energy as well as solvent environments, which leads to different interaction between photoproduct and solvent. This observation clearly demonstrates that solvent-solute interaction can modify and/or make a new reaction path that is not observed in the gas phase.

Poster Presentation : **PHYS.P-206**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Rebinding Dynamics of CO with Cytooglobin in Aqueous Solution Using Time-Resolved Vibrational Spectroscopy

JuHyang Shin, Manho Lim^{*}, CheongHa Lim¹

Department of Chemistry, Pusan National University, Korea

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Time-resolved vibrational spectroscopy was used to investigate the rebinding dynamics of CO to cytooglobin (Cgb) in the time range of femtosecond to microsecond after photodeligation of CgbCO in D₂O solution at 283 K. the stretching mode of the CO bound in CgbCO consists of three conformational bands (denoted to A₀, A₁, and A₃). The three bands show the same immediate bleach but their decay was different: the A₀ band (40% of the total initial bleach) reveals 3 ns decay but the A₁ and A₃ bands decay with a time constant of 260 ns, indicating that photodeligation of CgbCO proceeds on the femtosecond timescale and the geminate rebinding (GR) of CO to Cgb is dependent on the conformation of CgbCO. The stretching mode of CO photodeligated from CgbCO shows two bands in femtosecond to nanosecond timescales and becomes one bands with the pump-probe delay. The evolution of the photodeligated CO band was well described by CO band in the heme pockets, protein cavities, and in solution. When the kinetics of the photodeligated bands was modelled by combining with the kinetics of the conformational bound bands, the GR rate as well as the rate from the cavity to the heme pocket were dependent on the protein conformation. GR of two bands (A₁ and A₃) is similar to GR in myoglobin (Mb) but overall GR is much more efficient in Cgb due to the large contribution from A₀ conformation, indicating that Cgb also has the primary docking site-like structure found in Mb that suppresses GR by restraining ligand motion but the suppression appears to be not as efficient as Mb. Relatively fast GR of the A₀ conformation suggests that the binding of CO to the heme protein is very sensitive to the conformation of the protein.

Poster Presentation : **PHYS.P-207**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Triphenylamine Tetrasubstituted Heterocyclic Aromatic Organic Hole Transport Materials for Perovskite Solar Cell: A Computational Approach

Maebienne Anjelica Gapol, Sang Hee Lee, Dong Hee Kim*

Department of Chemistry, Kunsan National University, Korea

Perovskite solar cells (PeSC) has undergone numerous and rapid developments leading to an unprecedented 22.7% power conversion efficiency. Discovery of a more efficient and stable hole transport material (HTM) is one of the major tasks faced in improving PeSC. Triphenylamine derivatives have been applied in various electro-optical materials and have been used as HTM in perovskite solar cell. In this presentation, we investigated a variety of heterocyclic aromatic hydrocarbon central moieties with triphenylamine substituents as possible HTM for PeSC. Energy levels, absorption spectra and electrochemical properties of the derivatives were calculated using density functional theory and time-dependent density functional theory to give the best HTM design for PeSC.

Poster Presentation : **PHYS.P-208**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis, Characterization and toxicity evaluation of D-Glucuronic Acid Coated Cr₂O₃ Nanoparticles

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Department of Chemistry, Kyungpook National University, China

In recent years transitional metal oxide nanoparticles are extensively studied due to their wide range of applications in the field of physical, chemical and material sciences. Herein we report the synthesis of ultra-small and monodisperse chromium oxide nanoparticles through polyol method. Rhombohedral structure Cr₂O₃ nanoparticles with 2.05 ± 0.1 nm average diameter were characterized. Surface coating and metal – D-glucuronic acid bonding were confirmed from Thermo gravimetric analysis (TGA) and Fourier transform infrared spectroscopy (FT-IR). The size dependence optical property were studied from UV-Visible spectrophotometer. The toxicity test was carried in two cell lines DU145 and NCTC1469 and found to be non-toxic up to 500 μ M to both cell lines. The water proton relaxivities were studied to understand the possibility as MRI contrast agent.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Study of T_1 relaxation properties of Polyacrylic acid (PAA) coating ultrasmall Gd_2O_3 nanoparticles for MRI

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Department of Chemistry, Kyungpook National University, Korea

Magnetic resonance imaging contrast agents (MRI-CAs) distinguish normal and abnormal tissues inside the body through the differential contrast enhancement. For biomedical application MRI-CAs, nanoparticle should be highly water soluble, stable, non-toxic, and ultrasmall in particle size. In This work, we synthesized Gd_2O_3 nanoparticles coated by polyarylic acid ($M_w = 5100$ Da) to obtain stable nano colloids, in order to achieve high-performance in vivo T_1 MRI. The ligand PAA was directly coated on the nanoparticle surface. The colloidal suspension showed a high r_1 value of 31.0 and r_2/r_1 ratio of 1.2 and exhibited high contrast T_1 MR images.

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Ultrasmall Gadolinium Oxides Nanoparticles Coated Poly(Acrylic Acid)-RGD as Theragnostic Agent: MRI and Gadolinium Neutron Capture Therapy

Son-Long Ho, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

Theragnostic agents are compounds that able for both diagnosis and therapy of diseases, which provide more advantages than a single-modal agent. In this work, ultrasmall gadolinium oxides nanoparticles which were coated with poly(acrylic acid) and linear RGD showed excellent magnetic resonance imaging properties and cancer-targetting ability, due to the presence of RGD moiety. Furthermore, these Gd₂O₃ NPs are also applied for gadolinium neutron capture therapy (GdNCT) on human glioblastoma U87MG cells and showed good results both in vitro and in vivo. Herein, poly(acrylic acid)-RDG coated gadolinium oxide nanoparticles were synthesized and used as MRI and in vivo gadolinium neutron capture therapy agent (GdNCT) of human glioblastoma astrocytoma (U87MG) cells.

Poster Presentation : **PHYS.P-211**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

D-glucuronic acid-coated ultrasmall BiOI nanoparticles as potential X-ray contrast agent

Adibehalsadat Ghazanfari, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Iran

Until now there are many metal oxide nanoparticles that were synthesis for CT contrasting agents. In this work we studied D-glucuronic acid coated BiOI for CT contrast agent. The characterization result shows that all the particles are monodisperse in size, shape and highly crystalline in nature. By transmission electron microscopy, we measured diameter of nanoparticles. The average particle diameters of nanoparticles were estimated to be 1.85 nm .The structural, morphological, other properties, and their application are studied. The goal of this work is to examine the effect of the surface coating of bismuth oxyiodide nanoparticles. All the synthesized metal oxide nanostructures were characterized by transmission electron microscopy, powder X-ray diffraction and IR spectroscopy.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis and Characterization of PAA@Gd₂O₃ NPs as Multi-Purpose Therapeutic Agent

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Magnetic resonance imaging (MRI) has played a vital role in clinical diagnosis because of its high spatial resolution and great sensitivity. Besides, MRI can be used with remedial agent which is able for both diagnosis and therapy of disease. In this regard, gadolinium nanoparticles have great potential to act as therapeutic contrast agents. First of all, gadolinium ion (Gd(III)) has seven unpaired 4f electrons (8S_{7/2}), which generate large electron magnetic moment, also, Gd(III) efficiently induces the longitudinal relaxation of water protons. That makes Gd(III) the most suitable T₁ MRI contrast agent. Second, Gadolinium has high thermal neutron capture cross-section (), for example ¹⁵⁷Gd isotope has S-value of 254000 barnes, that is 60 times larger than the value of 10B, a commercialized agent for boron neutron capture therapy (BNCT). Therefore, gadolinium nanoparticles are preferable agent for neutron capture therapy of tumors. In this study, Gadolinium oxide nanoparticles coated with polyacrylic acid (PAA) -rhodamine B (Rho) 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-213**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication and characterization of ultrasmall C@Gd₂O₃ NPs as MRI agent and fluorescence imaging

Huan Yue, Gang Ho Lee*

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In the present study, for carbon coating we used carbohydrate(dextrose) to prepared the monodisperse and non-toxic ultrasmall carbon coated gadolinium oxide nanoparticles(C@Gd₂O₃ NPs) through a simple one-pot process in a solution. The C@Gd₂O₃ NPs to form stable colloidal suspensions in water and enhance biocompatibility, Besides, the C@Gd₂O₃ have a core-shell structure and a narrow size distribution in the range of 3nm±2nm. A clinical 1.5T MRI scanner was used to examine the longitudinal relaxivity (r₁). The resultant products can be used as T1 MRI contrast agent. Under the irradiation of UV light at 365 nm, the carbon nanoparticles show sky-blue color and show green color under Confocal Laser Scanning Microscope at 525nm. Therefore, C@Gd₂O₃ can be used as T1 MRI agent and fluorescent imaging.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis, characterization, and enhanced cancer-imaging of TAT-peptide conjugated ultrasmall Gd₂O₃ nanoparticles

Mohammad Yaseen Ahmad, Gang Ho Lee^{1,*}

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Trans-activator of transcription (TAT) peptide conjugated ultrasmall gadolinium oxide (Gd₂O₃) nanoparticles were synthesized using a one-pot process. The obtained nanoparticles were characterized by FT-IR, XRD and TEM. The average particle diameter of the GNPs was 1.5 nm. The cytotoxicity of the TAT peptide-GNPs was studied with cancer cell lines DU145 and NCTC1469. We measured in vivo T1 magnetic resonance (MR) images in a model nude mouse with liver cancer before and after to intravenous administration. The sample solution exhibited a longitudinal water proton relaxivity (r₁) of 18.2 s⁻¹mM⁻¹ (r₂/r₁ = 1.6, r₂ = transverse water proton relaxivity), which is 4 - 5 times higher than those of commercial Gd-chelates. This demonstrates the feasibility of using functionalized ultrasmall gadolinium oxide nanoparticles with uniform (~1.5 nm) sizes as an enhanced cancer-imaging agent similar to the cancer-targeting agent in T1 MR imaging (T1 MRI).

Poster Presentation : **PHYS.P-215**

Physical Chemistry

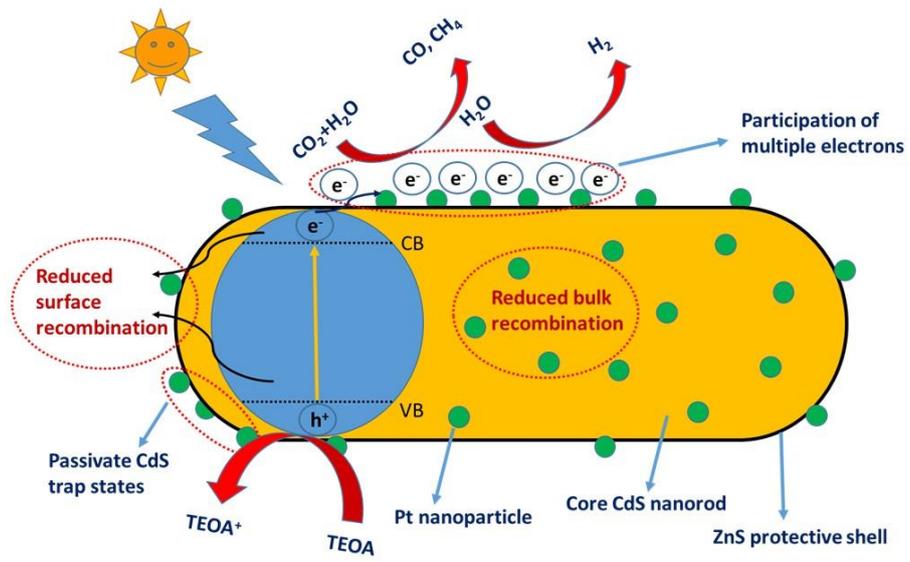
Grand Ballroom, FRI 11:00~12:30

Construction of 1-D ternary Nano hybrid CdS/ZnS/Pt for high selective CO₂ reduction with water- Highly efficient and durable semiconductor for CO generation

Praveen Kumar Dharani, Putta Rangappa, TaeKyu Kim*

Department of Chemistry, Pusan National University, Korea

Carbon dioxide (CO₂) the major contributor to climate change becoming increasingly apparent and worrisome due to its role as greenhouse gas. Conversion of anthropogenic (CO₂) to value-added chemicals through solar driven catalysis considered as an appealing approach to tackle CO₂ emission challenges. Although materials developed to produce high energy fuels from CO₂ reduction with water, it is still a challenge to develop suitable, highly efficient and stable nanostructures for long time operation. As CO₂ reduction reaction requires participation of multiple electrons, only nano hybrids involving two are more selective co-catalysts is beneficial. Herein, we report photo deposited Pt on core shell structured CdS-ZnS nano hybrid as durable catalyst for CO₂ reduction. The unique design integrates covering of CdS nanorods with ZnS shells and further photo reduction of H₂PtCl₆ onto CdS/ZnS in water-alcohol system. This delicate design accelerates the separation and transfer of photo generated charges, enhanced the photo absorption, reduced photo corrosion of CdS and facilitates abundant catalytic active sites. The as-synthesized CdS/ZnS/Pt nano hybrids are investigated for photocatalytic CO₂ reduction with water to produce CO and CH₄ in presence of Tri ethanol amine (TEOA) as hole (h⁺) scavenger. The optimized CdS/ZnS/Pt catalyst exhibited good stability for more than 42 hrs with unbroken rate of reaction for CO generation. The hybrid material realizes efficient solar-to-chemical energy conversion in suspension, demonstrating the potential of delicate structured materials are highly efficient and stable catalysts for photo reduction of CO₂.



Poster Presentation : **PHYS.P-216**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational studies of C_n Fullerenes (n=60, 70, 76, 84) and Photochemical Properties of Expanded Porphyrins

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Porphyrins and fullerenes donor-acceptor complexes are covalently linked in all these structures and adopt specific conformations that allow the π -electron systems to interact, even in the ground state. This has been attributed to strong van der Waals interactions. We calculated the Expanded Porphyrins (host 1,2) and complex Expanded Porphyrins: C_n Fullerenes (n=60, 70, 76, 84) using density functional theory (DFT) with a 6-31G(d) basis set. In order to include the solvent polarization effect was used in calculation for the Expanded Porphyrins (host 1,2) and complex Expanded Porphyrins: C_n Fullerenes (n=60, 70, 76, 84) in toluene and benzonitrile. After optimization, the absorption and frontier molecular orbitals (FMOs) for Expanded Porphyrins (host 1,2) and complex Expanded Porphyrins: C_n Fullerenes (n=60, 70, 76, 84) were carried out with the time dependent-density functional theory (TD-DFT), method using TD-M062X/6-31G+(d) level of theory.

Poster Presentation : **PHYS.P-217**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Effect of Co on Ni(OH)₂ Layered Double Hydroxide Nanosheets as High Charge Rate Capability and High Energy Density Storage Material in Ni-Zn Battery

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Improving the charge capacity, electrochemical reversibility and stability of anode materials are main challenges for the development of Ni-based rechargeable batteries and devices. The combination of cobalt and electrode material nanostructuration revealed a very promising approach for this purpose. Here we employed the controllable synthesis of nanosheet type NiCo LDH by electrodeposition method. The effect of concentration rate of Ni-to-Co preparation solution on crystalline structure, morphology, and supercapacitive performance was investigated systematically. Experimental found that the morphology and composition of NiCo LDH was highly depend on the Ni²⁺/Co²⁺ molar ratios and the obtained Ni_{0.9}Co_{0.1} LDH materials showed small nanosheet size and uniform distribution on carbon fiber electrode. Ni_{0.9}Co_{0.1} LDH electrode was evaluated for half-cell battery application, which revealed a high specific capacity of 278 mAh. g⁻¹ at C/5 charge rate and a good cycle stability, retaining 80% of the initial capacitance after 120 charge and discharge cycles at 1C charge rate. Moreover, the Ni_{0.9}Co_{0.1} LDH electrode exhibits a high energy density of 228 Wh Kg⁻¹ at a power density of 55.6 W Kg⁻¹ and a high power density of 1020 W Kg⁻¹ at energy density of 135.5 Wh Kg⁻¹ within a 1.63 V of Ni_{0.9}Co_{0.1}-Zn battery.

Poster Presentation : **PHYS.P-218**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Few layered Pervoskite $\text{Ba}_2\text{NbFeO}_6$ nanostructures deposited on exfoliated $\text{g-C}_3\text{N}_4$ Nanosheets as Efficient Catalysts for Hydrogen Evolution

Praveen kumar Dharani, Amaranatha Reddy, TaeKyu Kim*, EunHwa Kim

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Two dimensional materials play a major role in state-of-the-art innovations for energy conversion because of potential applications resulting from their unique properties. These materials additionally show inordinate potential towards the progress of hygienic power sources to deal with increasing environmental disputes at a time of skyrocketing energy demands. Herein, we report earth-abundant, few-layered, $\text{BaNbFeO/gC}_3\text{N}_4$ nanocomposites, which reduce photogenerated electron and hole recombination by effectively separating charge carriers to achieve a high photocatalytic efficiency. Accordingly, the $\text{BaNbFeO/gC}_3\text{N}_4$ system produced effective hydrogen ($1,600 \mu\text{mol}\cdot\text{h}^{-1}$) as of water using $\text{Na}_2\text{S/Na}_2\text{SO}_3$ aqueous solution with the irradiation of solar-light. The presence of few-layered BNFO in gC_3N_4 successfully separates photogenerated charge carriers, thereby enhancing shuttling of electrons on the surface to active edge sites. To the best of our knowledge, this few-layered $\text{BaNbFeO/gC}_3\text{N}_4$ system exhibits the most effective concert among altogether reported gC_3N_4 based materials. Notably, these findings will ample prospective for the development of enormously real photocatalytic systems due to its economically viable and extraordinary efficiency.

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Atomistic Insights into the Thermo-Mechanical Properties and Li Diffusion in ψ -Graphene for Lithium-Ion Battery Anode Material

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Developing cleaner and sustainable energy still remains as one of the biggest challenges of this century. By employing classical molecular dynamics simulations, we investigated the structural, thermo-mechanical, and Li-ion diffusion properties of ψ -graphene (ψ -graphene), which is a planar two-dimensional (2D) defect-filled membrane akin to graphene.¹ The fairly high specific heat capacity of ψ -graphene is interpreted as a signature of strong anharmonicity in the material and also serves to prevent the possibility of thermal runaway in Li-ion batteries upon overheating. Although the Young's moduli of ψ -graphene are smaller than graphene,² it possesses high in-plane stiffness which helps to prevent possible volume expansion upon Li intercalation, which is a major drawback of silicon-based anodes. The obtained low Li-ion migration activation energy (< 0.16 eV) ensures the presence of fast ion conduction in ψ -graphene, with a room temperature diffusion coefficient $1.11 \times 10^{-9} \text{cm}^2/\text{s}$, which strongly suggests favourable electrode kinetics. These properties make it as a promising and extraordinary anode material for use in Li-ion batteries (LIBs) with fast charge/discharge rates. References 1. Li, X.; Wang, Q.; and Jena, P. ψ -Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries *J. Phys. Chem. Lett.* 2017, 8, 3234-3241. 2. Thomas, S.; Ajith, K. M.; Lee, S. U.; and Valsakumar, M. C. Assessment of the mechanical properties of monolayer graphene using the energy and strain-fluctuation methods. *RSC Adv.*, 2018, 8, 27283-27292.

Poster Presentation : **PHYS.P-220**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaporation of hydrogen-bonded guanine dimers upon collisional activation of Na⁺-bound G-quartets

Yoonkyung Choi, Sang Yun Han*

Department of Nano Chemistry, Gachon University Global Campus, Korea

Na⁺-bound G-quartets exhibits intriguing square planar structures formed by non-covalent interactions including ion-dipole interactions and multiple hydrogen bonding. In this study, energy-resolved collision-induced dissociation (ER-CID) of Na⁺-bound complexes of G-quartets with mixed ligands of guanine (G) and 9-methylguanine (9mG), [Na·G_m·9mG_n]⁺ (m + n = 4) were investigated using tandem mass spectrometry in a combined approach with quantum chemical calculations. Theoretical study suggested that all five Na⁺-bound G-quartets investigated in this study possess square planar structures. The mass spectrum of [Na·G_m·9mG_n]⁺ produced by electrospray ionization (ESI) exhibited generation of mixed clusters of Na⁺-bound dimers and G-quartets, wherein Na⁺-bound trimers (m + n = 3) were essentially missing. In addition, CID of G-quartets hardly produced fragments of Na⁺-bound trimers from the square planar complexes, while formation of dimeric fragments was pronounced. These suggest that a great stability is achieved by forming a complete hydrogen bonding network in G-quartets, which agrees well with a large predicted stepwise enthalpy gained by complexation with the fourth ligand, which is as high as 55 kcal/mol. The stability by hydrogen bonding network between G moieties in G-quartets further suggests that Na⁺-bound dimeric fragments may arise from neighboring, hydrogen-bonded ligands; it allowed to address the stereochemistry of G-quartets, of which population for *cis*- and *trans*-conformers of [Na·G₂·9mG₂]⁺ can be assessed to be 50:50 in the gas phase. The ratio of 50:50 also suggests that the G-quartets were likely to be formed in the solution due to thermochemical stability rather than in the course of electrospray ionization via kinetic trapping.

Poster Presentation : **PHYS.P-221**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational Study on Structure, Dynamics, and Aggregation of A β 42 protofibril

MinJun Lee, Jeseong Yoon*, Seokmin Shin*

Department of Chemistry, Seoul National University, Korea

Amyloid proteins are related to neurodegenerative diseases especially as a main symptom of amyloid fibril deposit in neuronal cell of patients brain. A β is known to be the major cause of Alzheimer's disease. It is suggested that A β 42 is more toxic than A β 40. It is possible that the higher toxicity is due to its conformational features. Therefore it is worth to examine the structural features in this viewpoint. Luhrs suggested U-shaped β -arch structure of A β 42 in 2005, and more recently Xiao succeeded in obtaining high-resolution solid state NMR structure of A β 42 which is unexpected S-shaped triple- β structure in 2015. Although some experiments provide valuable informations on fibril structure of A β 42, we need to observe different aspects of structural informations, that is, dynamic and thermodynamic properties of fibril structure as well as its interaction with water in order to explain conformational stability and aggregation mechanism in relation to structure of A β 42 fibril. We performed molecular dynamics simulations on two different A β 42 models: U-shaped β -arch and S-shaped triple- β structures. In order to examine both structural stability and aggregation pathway, we performed several different simulation methods which are straightforward extensive simulation, steered molecular dynamics, and replica exchange molecular dynamics (REMD). By analyzing the simulation trajectories, we clarified the structural features of A β 42 protofibril motif and related them to the stability of fibril. From these results, we tried to interpret the trajectories of pulling simulation and REMD and predict aggregation pathway of A β 42 fibril.

Poster Presentation : **PHYS.P-222**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The role of proton transfer in collision-induced dissociation of proton-bound hetero dimers of nucleic acid bases in the gas phase

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¹*Department of Nano Chemistry, Gachon University Global Campus, Korea*

We report the role of proton transfer in the proton-bound hetero dimers of C (cytosine), 1-MeC (1-methylcytosine), 5-MeC (5-methylcytosine) with G (guanine), and 1-MeG (1-methylguanine), 7-MeG (7-methylguanine), and 9-MeG (9-methylguanine) with 1-MeC. In the results, CID of proton-bound Hoogsteen base pair $C:H^+\cdots G$, exhibited more abundant production of $C:H^+$, the fragment protonated on the moiety with a smaller proton affinity, than $G:H^+$. This appeared to contradict general prediction based on the kinetic method. However, further theoretical exploration of potential energy surfaces found that there can be facile proton transfers in the proton-bound Hoogsteen base pairs during the CID process, which makes the process accessible to an additional product state of O-protonated C for $C:H^+$ fragments. The presence of an additional dissociation channel, which in other words corresponds to 2-fold degeneracy in the transition state leading to $C:H^+$ fragments, effectively doubles the apparent reaction rate for production of $C:H^+$. In this way, the process gives rise to the anomaly, the observed pronounced formation of $C:H^+$ in the CID of the proton-bound Hoogsteen base pair, $C:H^+\cdots G$. In this study, the effects of proton transfer that affect dissociation channels are extensively examined using various methylated guanines.

Poster Presentation : **PHYS.P-223**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

DFT study into subnanometer cobalt clusters interaction with pristine/defective graphene: Nucleation and HER activity

Jun Ren, Nasir Shahzad, Chan Kyung Kim*

Department of Chemistry & Chemical Engineering , Inha University, Korea

The cobalt nanoparticles adsorbed on graphene are new catalysis systems of interest for Fischer-Tropsch synthesis (FTS) to obtain clean fuel hydrocarbons. Graphene decorated with Co nanoparticles, especially, could be a nice alternative material for catalysis in CO+H₂ reaction. On the basis of first-principles calculation, we have analysed the binding of Co_n cluster (n=1-7) with pristine (PGr) and defective (DGr) graphene. Our analysis shows that the electronic structure of the graphene-supported Co subnano-clusters based on metal-support interactions plays a significant role in the catalytic activity, and the interaction between the Co_n clusters and the graphene is rather local. Our results also show that the bigger the size of Co_n clusters, the smaller the interaction between the clusters and the supports, and thus the lower its structural distortion. In addition, the nucleation of Co_n clusters on PGr is thermodynamically favourable, but the opposite trend was obtained on DGr. Both the pristine and defective surfaces facilitate agglomeration of Co₆ cluster, implying that the graphene support remarkably promotes and even prevents the sintering process of small Co clusters. The Bader charge also showed that both Cobalt and graphene support are responsible for the charge state of Co clusters. In addition, the HER activity on the Co_n/PGr and Co_n/DGr systems have been examined by H adsorption calculations. The good HER catalytic behaviour of Co_n/graphene system is proved to be the best HER catalyst embedded in defect lattice sites of graphene.

Poster Presentation : **PHYS.P-224**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Detecting Low Concentrations of Unsaturated C-C Bonds by Parahydrogen-Induced Polarization using an Efficient Home-Built Parahydrogen Generator

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Parahydrogen has great potential as a hyperpolarization source. To achieve the hyperpolarized parahydrogen, heat exchanger in ultra-low temperature is the essential part and low temperature is normally sustained by wasteful liquid nitrogen. To save the liquid nitrogen in this home-built parahydrogen generator, we utilized the cryogenic storage dewar and it lasted more than 20 days in a single fueling. A principle-based experiment, identifying small concentration of unsaturated bond compound in mixture by using hyperpolarization and phase difference, was carried out by hydrogenation reaction. Lower than 1 μ l styrene in 1 ml chloroform was identified by a single scan of 43 MHz Benchtop NMR after hydrogenation reaction via 50% parahydrogen. This method could be developed with great potential such as using high field NMR, higher parahydrogen concentration, and more scan time to collect data etc. Because hydrogenation reaction by parahydrogen induce reversed phase in attaching on the unsaturated C-C bond, many other unsaturated bonds in organic molecules might be used for detection. This study will not only broaden the parahydrogen-based unsaturated bond detecting study but also hyperpolarization study on many researchers by providing the long time lasting system of home-built parahydrogen generator

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

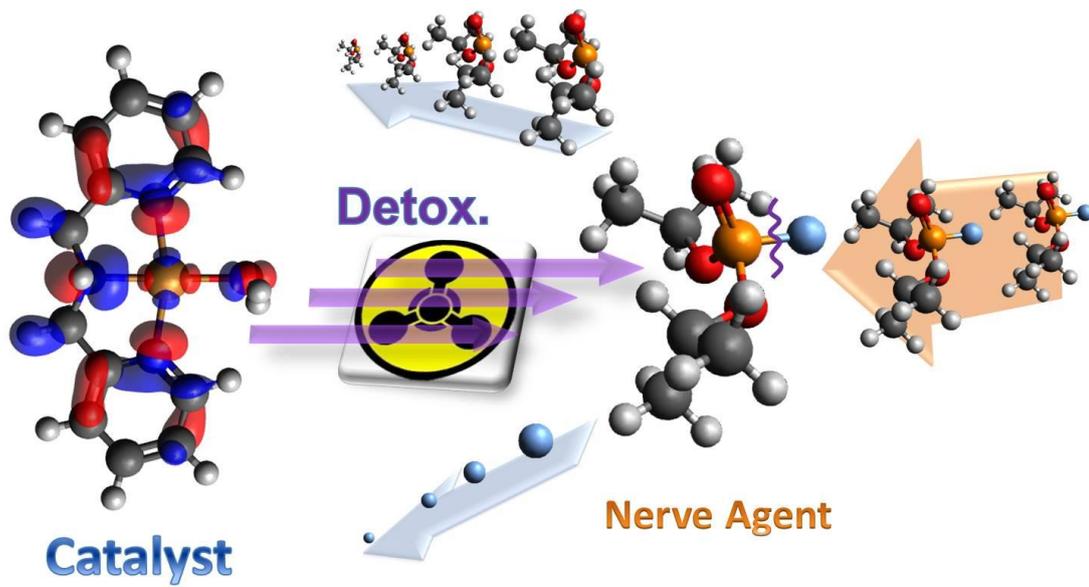
Diisopropyl fluorophosphate (DFP) degradation activity using transition metal–dipicolylamine complexes

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Department of Chemistry, Korea Military Academy, Korea

¹*Korea Military Academy, Korea*

Transition metal complexes have been extensively used as catalysts for organophosphorus agent decomposition to reduce their toxicity with their performance being strongly dependent on the nature of the metal ion. To investigate this dependence, we prepared dipicolylamine (DPA)-containing complexes of Cu(II), Zn(II), Ni(II), Co(II), and Fe(II) and analyzed their activities for the degradation of diisopropyl fluorophosphate (DFP), a nerve agent surrogate compound. Cu(II)-DPA complex showed fastest reaction kinetics while Zn(II)-DPA and Ni(II)-DPA exhibited more slower reactions. This observation can be explained using frontier molecular orbital (FMO) theory, which revealed that the nucleophilicity of the oxygen atom in water molecules in these transition metal complexes was well matched with reactivity order observed in experiments. These investigations combined with theoretical study provide valuable information for designing and predicting the activity of new transition metal-organic ligand complexes as a catalyst to decompose and reduce toxicity of organophosphorus nerve agents.



Poster Presentation : **PHYS.P-226**

Physical Chemistry

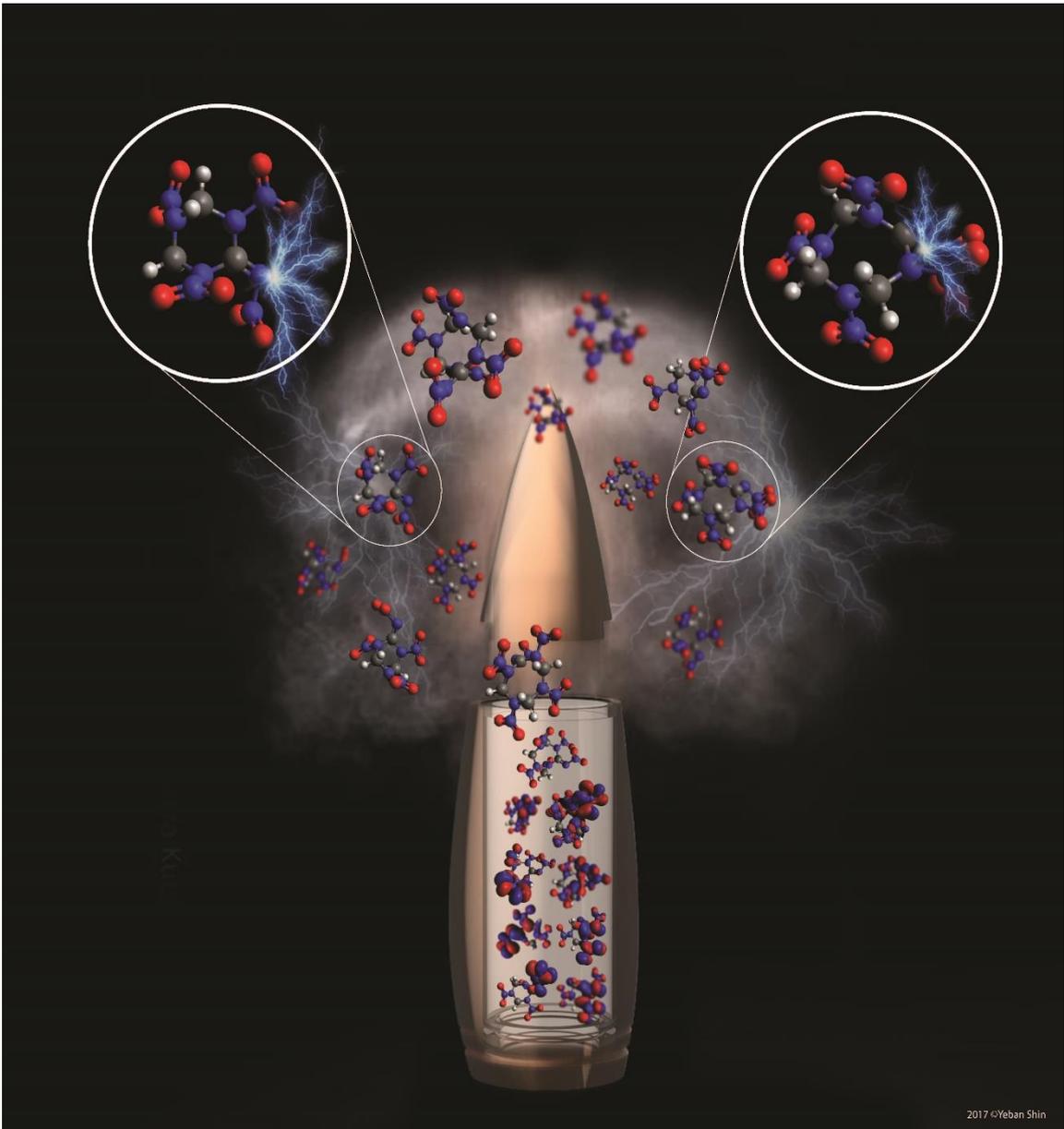
Grand Ballroom, FRI 11:00~12:30

New Theoretically Predicted RDX- and β -HMX-based High-Energy-Density Molecules

Keunhong Jeong

Department of Chemistry, Korea Military Academy, Korea

Theoretically new high-energy and -density materials (HEDM) in which the hydrogens on RDX and β -HMX (hexahydro-1,3,5-trinitro-1,3,5-triazine and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, respectively) were sequentially replaced by (N-NO₂)_x functional groups were designed and evaluated using density functional theory (DFT) calculations in combination with the Kamlet-Jacobs equations and an atoms-in-molecules (AIM) analysis. Improved detonation properties and reduced sensitivity compared to RDX and β -HMX were predicted. Interestingly, the RDX and β -HMX derivatives having one attached N-NO₂ group [RDX-(NNO₂)₁ and HMX-(NNO₂)₁] showed excellent detonation properties (detonation velocities: 9.529 and 9.575 km·s⁻¹, and detonation pressures: 40.818 and 41.570 GPa, respectively), which were superior to the parent compounds. Sensitivity estimations obtained by calculating impact sensitivities and HOMO-LUMO gaps indicated that RDX-(NNO₂)₁ and HMX-(NNO₂)₁ were less stable than RDX and HMX but more stable than any of the other derivatives. This method of sequential NNO₂ group attachment on conventional HEDMs offers a firm basis for further studies on the design of new explosives. Furthermore, the newly found structures may be promising candidates for better HEDMs.



Poster Presentation : **PHYS.P-227**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Density Functional Theory Study on the Reactivity of Anti-oxidants toward DPPH

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Department of Chemistry and Chemical Engineering, Inha University, Korea

DPPH is an abbreviation for the organic compound 2,2-diphenyl-1-picrylhydrazyl. It is a dark-coloured crystalline powder composed of stable free-radical molecules. DPPH is widely used in a laboratory experiment to monitor chemical reactions involving radicals, most notably in a common antioxidant assay. Many food ingredients contain polyphenol compounds, such as vitamin C, vitamin E, gallic acid, salicylic acid, quercetin, and kaempferol. In this work, the relative reactivity of these compounds toward DPPH was examined by the density functional theory (DFT) using the B3LYP/6-31G(d,p) level of theory. All the structures were optimized using Gaussian 16 package and were verified as minima with positive frequencies or as a transition state with one imaginary frequency. As there are many possible sites for proton abstraction in each compound, all the possible pathways were examined. One of the products of the reaction is another reactive radical, which will further complicate the interpretation of reactivity data.

Poster Presentation : **PHYS.P-228**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Characteristic of a CNT Sponge Preconcentrator for GC Analysis of VOCs in Air Samples

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A miniature on-line sorption trap is used to preconcentrate volatile organic compounds (VOCs) from large-volume air samples and inject the organic compounds into the separation column of GC as a relatively narrow vapor plug. The CNT sponge adsorbents were assessed on the basis of analyte thermal-desorption bandwidth and efficiency, chromatographic peak shape, and breakthrough volume against mixtures of organic compounds. The determination of a vapor mixture of common air contaminants in

Poster Presentation : **PHYS.P-229**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Fluorescence modulation near Ag nanopores of different pore diameters

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Nanoporous metals provide unique nanoscopic environment to enhance fluorescence of adjacent fluorophores. Accumulated optical fields in nanopores can enhance absorption process of fluorophores therein and subsequently accelerate radiative recombination. According to the theory, metal-enhanced fluorescence (MEF) can be modulated by a function of nanopore diameter. In this study, we prepared the nanoporous Ag skeletons by reduction-induced decomposition (RID) process of AgCl. The RID process simply controls the pore diameter of the resulting nanoporous Ag skeletons. It was revealed that MEF efficiency is enhanced in the nanoporous Ag with the smallest nanopore size, whereas the larger porous Ag skeletons severely quench emission. This experiment is carefully studied with time- and space-resolved fluorescence microscopy.

Poster Presentation : **PHYS.P-230**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Precise evaluation of carrier dynamics and photo-stability of binary perovskite by emission lifetime imaging

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Daegu Center, Korea Basic Science Institute, Korea

Perovskite materials have attracted tremendous attention because of its high solar energy conversion efficiency. Recently, binary and ternary perovskite phases have been studied to control band-gap energy in the full visible range. It is still a challenging study to prepare homogeneous phased perovskite materials. Hence, there is increasing needs on the precise characterization of spectroscopic information. Here, we used photoluminescence lifetime imaging (PLIM) spectroscopy for studying the carrier dynamics and photo-stability of binary perovskite materials. The PLIM technique precisely evaluates the carrier dynamics of pure and phase segregated materials by emission spectrum and lifetime at a nanoscopic area.

Poster Presentation : **PHYS.P-231**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Few layered black phosphorus/MoS₂ nanohybrid: A promising co-catalyst for solar driven hydrogen evolution

Amaranatha Reddy, EunHwa Kim, Madhusudana Gopannagari, Yujin Kim, Praveen Kumar Dharani, TaeKyu Kim*

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Exploring active and stable photocatalysts is an essential requirement for boosting the efficiency of photocatalytic water splitting to obtain clean hydrogen fuel. Here, a few layered black phosphorus/MoS₂ (BP-MoS₂) nanohybrid was successfully prepared and verified it for photocatalytic hydrogen evolution using CdS nanorods as light absorbers. The resulting nanohybrids manifest remarkable catalytic performance with high amount of H₂ production (CdS/BP-MoS₂: 183.24 mmol h⁻¹ g⁻¹) and outstanding catalytic stability. The observed amount of H₂ is much higher than that of various CdS/BP and CdS/MoS₂ based nanohybrids reported earlier. We expect that the demonstrated new heterostructured design strategy may bring novel insights to develop low-price noble metal free photocatalysts for hydrogen evolution. Key words: Photocatalytic hydrogen evolution, co-catalysts, reduced recombination, cadmium sulfide, black phosphorus.

Poster Presentation : **PHYS.P-232**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Heating stability observation of binary and quaternary blend organic photovoltaics via *in situ* photoluminescence spectroscopy

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Organic photovoltaics (OPV) are remarkable solar cell because its processability and competitive price. Performance of OPV is directly related to its power conversion efficiency (PCE), which depends on state of bulk heterojunction in device. Bulk heterojunction of OPV is commonly binary blend (b-OPV), one component is conjugated polymer (electron donor) and the other is fullerene derivative (electron acceptor). Unfortunately, the PCE of these ordinary OPV rapidly decreases in heating condition. Recent researches show that using quaternary blend (q-OPV) composed of two different electron donors and two similar electron acceptors can increase thermal stability of OPV. However, *in situ* spectroscopic studies to interpret this phenomenon on a molecular level are insufficient until now. Here we show that *in situ* spectroscopic data obtained by using home-built Raman spectrometer. In both Raman spectra of b-OPV and q-OPV, degradation of conjugated polymers was not observed. Interestingly, generation of fluorescence was observed in b-OPV, but not in q-OPV. It is known that fullerene derivatives can act as fluorescence quencher, so this spectroscopic difference may be related to state of electron acceptors. Accordingly, we concluded that mobility of electron acceptors and morphological state in the b-OPV are more affected by heating than those in the q-OPV. We hope that this research will help an improvement of thermal stability of OPV.

Poster Presentation : **PHYS.P-233**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

[Withdrawal] Temperature dependence of Rhodamine B coated upconversion nanoparticles in the presence of glutathione

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Korea*



Poster Presentation : **PHYS.P-234**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational Approach for Thermally Activated Delayed Fluorescence of *Nido*-Carboranes

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Organic light emitting diodes (OLEDs) are promising for the next generation displays and lighting due to their low power consumption and potentially long operational lifetime. Thermally activated delayed fluorescence (TADF) materials have recently attracted great attention as efficient emitters in OLEDs.¹ TADF emitters are intrinsically pure organic materials, which can harvest triplet excitons via reversed intersystem crossing (RISC). To facilitate RISC within a practically reasonable temperature range, TADF emitters require a very small energy difference (ΔE_{ST}) between the excited singlet (S_1) and triplet states (T_1). This is usually achieved by constructing TADF emitters with rational molecular designing, allowing the structures for effective reduction in the spatial overlap between HOMO and LUMO. Hence, it remains quite challenging to search for an appropriate combination with proper molecular configuration with donor and acceptor moieties to attain excellent TADF activity. In this presentation, a theoretical insight into the ΔE_{ST} of the new class of donor family (*nido*-carboranes) will be discussed. In addition, how the TADF activity can be used as a sensitizer will be mentioned along with the TADF activity of triarylboron (TAB) compounds.² [References: 1.H. Uoyama, K. Goushi, K. Shizu, H. Nomura and C. Adachi, *Nature*, 2012, **492**, 234.; 2.N. V. Nghia, S. Jana, S. Sujith, J. Y. Ryu, J. Lee, S. U. Lee and M. H. Lee, *Angew. Chem. Int. Ed.*, 2018, (just accepted manuscript)]

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaluation of thermal hysteresis activity of ice-binding protein using molecular dynamics simulation

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

Ice-etching experiment and molecular docking demonstrated that two ice-binding proteins (IBP), LeIBP from arctic yeast and FfIBP from sea ice bacterium, show different activities in suppressing the growth of ice, leading to different thermal hysteresis (TH) even though they share common features in primary/tertiary structures. In this study, we investigated the ice-binding pattern of the two IBPs to different ice planes, prism and basal plane using all-atom molecular dynamics simulation. Our results provide a fully atomistic description of the difference in TH of two IBPs.

Poster Presentation : **PHYS.P-236**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Gas Preconcentrator Based on Carbon Nanotube Sponge for VOCs Detection

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A small CNT sponge preconcentrator for the GC analysis, designed to determine complex mixtures of volatile organic compounds (VOCs), is described. CNT sponges were synthesized by CVD process using ferrocene and 1,2-dichlorobenzene as the catalyst precursor and carbon source, respectively. The sponge morphology and CNT structure was characterized by SEM, TEM, EDS, XPS, and Raman. CNT sponges cut into a rectangular block ($3 \times 2 \times 45 \text{ mm}^2$, 5mg) was inserted between metal frits in a 1/4" Quartz tube. After sample trap by the adsorbent, the flow direction through the preconcentrator is reversed, and the thermally desorbed analyte is directly introduced into the GC capillary column module. Preconcentration factor of greater than 100 is observed for VOCs compounds.

Poster Presentation : **PHYS.P-237**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Rotational spectra and conformations of 2-bromo-1-butene using Fourier-transform microwave spectroscopy

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Department of Chemistry, Sookmyung Women's University, Korea

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Microwave spectra of 2-bromo-1-butene ($\text{CH}_2=\text{CBrCH}_2\text{CH}_3$) were measured by a chirped-pulse and a resonant cavity Fourier-transform microwave spectrometer. Using GAUSSIAN09, *ab initio* calculations were performed for all three possible conformations, $d(\text{C1C2C3C4}) = 0^\circ$ (*trans*), 113° (*gauche*), and 180° (*cis*). Rotational transitions in the range of 2-19 GHz were assigned for the *trans* and *gauche* conformer, and the *cis* isomer were not observed. Rotational constants, centrifugal distortion constants, and nuclear quadrupole coupling constants were determined for ^{79}Br and ^{81}Br isotopologues of the *trans* and *gauche* conformer, respectively. In addition, the principal coordinates of bromine atom for two conformers were determined from the isotopic shifts. Spectroscopic constants and the coordinates are compared with and in good agreement with calculated values."본 연구는 환경부 「기후변화특성화대학원사업」의 지원으로 수행되었습니다." "This work is financially supported by Korea Ministry of Environment(MOE) as 「Graduate School specialized in Climate Change」."

Poster Presentation : **PHYS.P-238**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

First-Principles Study of Two-Dimensional Planar Carbon Allotropes for Lithium-Ion Battery Anode Materials

Siby Thomas, Hoijung Jueng, Byeongsun Jun, Sang Uck Lee*

Department of Bio-Nano Engineering, Hanyang University, Korea

One of the biggest challenges of this century is filling the gap between energy supply by developing a cleaner, sustainable and inexpensive energy. Herein, based on first-principles density functional theory (DFT) calculations, we systematically investigated the structural, electronic, mechanical and lithium (Li) ion diffusion properties of 2D defected graphene-like planar carbon allotropes (ψ -graphene,¹ pha-graphene,² haeckelite structures³ containing 5-, 6- and 7- membered carbon rings called h567, o567 and r57). Our calculations show that the 2D carbon allotropes possess significant structural and electronic stability with high metallicity which provided enhanced conductivity for Lithium-ion battery (LIB) application. We have calculated all the possible Li-migration paths in all the allotropes with a low and high state of charge (SOC). At high SOC, the Li migration barrier (E_a) is decreased to rather a small value,⁴ whereas the low SOC state shows nearly similar migration barrier comparable to graphene ($\sim 0.25 - 0.40$ eV). The obtained higher binding energy and low diffusion barrier of pha-graphane ($E_a \sim 0.11$ eV) and o567 ($E_a \sim 0.13$ eV) at high SOC configuration indicating the superiority of these allotropes as an electrode material in LIBs. In view of these excellent properties, our work predicts that pha-graphane and o567 can be promising anode materials for the development of low-cost high-performance LIBs. References: (1) Li, X. Y.; Wang, Q.; Jena, P. *J Phys Chem Lett* 2017, 8 (14), 3234-3241. (2) Wang, Z. H.; Zhou, X. F.; Zhang, X. M.; Zhu, Q.; Dong, H. F.; Zhao, M. W.; Oganov, A. R. *Nano Lett* 2015, 15 (9), 6182-6186. (3) Terrones, H.; Terrones, M.; Hernandez, E.; Grobert, N.; Charlier, J. C.; Ajayan, P. M. *Phys Rev Lett* 2000, 84 (8), 1716-1719. (4) Liu, J. Y.; Wang, S.; Sun, Q. *Proc Natl Acad Sci USA* 2017, 114 (4), 651-656.

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Charging/Discharging Characteristics of a Static Cell with Zinc and Poly-bromide Species

Joo-Hee Lim, Kyungmi Kim, Junghyun Chae, Cheol-Woo Yi*

Department of Chemistry, Sungshin University, Korea

The use of fossil fuels has been recently restricted because it has brought out environmental problems such as climate change, acid rain, and air pollution. Hence, the renewable resources including sunlight, wind, and geothermal heat have been utilized for replacement of fossil fuels. Due to the limitation of renewable energy like intermittency, however, energy storage system (ESS) has been developed to store electrical energy produced by renewable energy sources. Despite many efforts, ESS still needs to overcome its shortcomings as aspects of cost, longevity, and capacity to store energy. In our previous study, we prepared new static poly-bromide battery system and confirmed that poly-bromide species containing excess amount of bromine show higher discharge capacity with respect to the cell consisting of aqueous bromine. We correlated the discharge capacity of the static poly-bromide cell as a function of the amount of bromine in poly-bromide species determined by attenuated total reflection-infrared (ATR-IR) spectroscopy. In this study, continuing the previous study, we conducted electrochemical charging/discharging reaction to obtain stable operation and good performance. The poly-bromide species employing in this study were various equivalents of MEP-Br_x (0.39 – 2.34 equivalents) and we investigated electrochemical and physico-chemical properties as well as Coulombic efficiency (CE) and energy efficiency (EE). Moreover, we have investigated the poly-bromide species by various spectroscopic tools as a function of the number of charging/discharging cycle and correlated between the spectroscopic and electrochemical data.

Poster Presentation : **PHYS.P-240**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Few layered WSe₂ Nanosheets anchored on CdS nanorods for efficient hydrogen production under solar light irradiation.

**Kethireddy Arun Joshi Reddy, Amaranatha Reddy, Praveen Kumar Dharani,
Madhusudana Gopannagari, Putta Rangappa, Hwan Lee, TaeKyu Kim***

Department of Chemistry, Pusan National University, Korea

Transition Metal Dichalcogenides (TMDs) have recently attracted considerable attention, because of their interesting electrical, optical, mechanical and catalytical properties. Among different TMDs, here we synthesized Few layered WSe₂ nanosheets through a facile, low-cost and one-pot solvothermal method. Few layered WSe₂ nanosheets anchored on CdS semiconductor (FW/CdS) composite was synthesized by a simple ultrasonic method. The prepared Nano-composite was further characterized via XRD, XPS, SEM, TEM, DRS UV-Vis, photoluminescence. The mechanism has been investigated by Mott-Schottky and photoelectrochemical measurements. Under controlled experimental conditions, the synthesized FW/CdS composite generates high rate of H₂ production (103.5 mmol g⁻¹ h⁻¹) compare with bare CdS, bare WSe₂ and bulk WSe₂/CdS under solar light irradiation. The enhanced photocatalytic performance of Few layered WSe₂ is due to its porous nanostructure with many exposed active edge sites which provide large number of active reaction sites. As far as we know this is highest H₂ yield rate achieved by WSe₂-CdS photocatalyst under solar light irradiation.

Poster Presentation : **PHYS.P-241**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Self-Assembled Monolayers of Aromatic Selenocyanates with Methylene Spacer on Au(111) Prepared by Ambient-Pressure Vapor Deposition

Seul-ki Han, Jaegeun Noh*

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Aromatic selenolate self-assembled monolayers (SAMs) on gold substrate (or other metal substrates) have been extensively studied due to their various potential applications such as a biosensor, molecular electronics, and electronic interfaces. Also, aromatic SAMs with methylene-spacer between aromatic ring and headgroup have higher packing density and few defect densities than aromatic SAMs with only a benzene ring due to the flexibility of methylene. In this study, to determine dependence of the number of methylene spacer on the formation and structure of the SAMs, we investigated the SAMs of (2-selenocyanatoethyl)benzene (2-SCEB), (3-selenocyanatopropyl)benzene (3-SCPB), and (4-selenocyanatobutyl)benzene (4-SCBB) on Au(111) by scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). STM measurements showed a large difference in surface morphology of three SAMs of 2-SCEB, 3-SCPB, and 4-SCBB on Au(111) from vapor deposition at various temperatures and deposition times. 2-SCEB SAMs have vacancy islands (VIs) and ordered domains with domain boundaries, and optimized 2-SCEB SAMs have a ($\sqrt{3} \times 3\sqrt{3}$) packing structure at 363 K for 1 h. 3-SCPB SAMs have VIs and row-phase without domain boundaries, and the row-phase of SCPB SAMs have short bright lines at 348 K and 363 K. 4-SCBB SAMs have ordered domains with clear domain boundaries and small round VIs at 323 K, and the 4-SCBB SAMs show row-phase with long bright lines and disappear the domain boundaries at 348 K and 363 K. XPS result indicates that these selenolate SAMs were formed via cleavage of Se-CN bond from $\text{Ar}(\text{CH}_2)_n\text{Se-CN}$.

Poster Presentation : **PHYS.P-242**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Understanding Charge-Transfer Mechanism of Ag@Cu₂O Nanoparticles

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¹*Department of Chemistry, Jilin Normal University, China*

Charge-transfer mechanism (CT) has recently been investigated due to its shows great enhancement effect on the surface-enhancement Raman scattering. To understand the CT mechanism, semiconductor materials are very useful because they have band gap between valence band and conduction band. Especially, Cu₂O has the advantage that the Raman enhancement through CT is superior to other p-type semiconductor materials because the band gap of Cu₂O is more narrow than the other. In this study, we examined the CT mechanism between Cu₂O and para-aminothiophenol (PATP) of PATP absorbed on Ag@Cu₂O, by using UV-Vis, TEM, XPS and Raman spectroscopy. Details on analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-243**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Understanding surface reaction between LiFePO_4 electrode-electrolyte interface using *in situ* Raman spectroscopy

Soo Min Kim, Yeonju Park, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

Nowadays, demands for use in electric vehicles, portable devices and batteries as storage of renewable energy are increasing. Among the Li-ion batteries, iron-based cathode material such as LiFePO_4 is low cost and has long cycle life, high thermal stability and environmental friendliness. Thus, we made Li-ion battery used LiFePO_4 cathode material in this study. In this study, we performed *in-situ* Raman spectroscopy and electrochemical performance during battery operation to explore surface change mechanisms of the LiFePO_4 cathode. In this presentation, the details of our work will be discussed.

Poster Presentation : **PHYS.P-244**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The denaturation mechanism of α -lactalbumin by pH-dependent fluorescence spectroscopy and PARAFAC analysis

Yujeong Park, Yeonju Park, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

It is important to study the protein denaturation process because it can provide fundamental knowledge in the study of disease caused by protein denaturation. α -Lactalbumin, a representative whey protein, has an intermediate state (or molten globule state) under various conditions, such as low pH, heating, and in the presence of chemical denaturants. In this study, the pH-induced denaturation mechanism of α -lactalbumin was investigated by fluorescence spectroscopy. Principal component analysis (PCA) was used to understand the denaturation mechanism of α -lactalbumin. Parallel factor analysis (PARAFAC) was used to decompose the residues of α -lactalbumin. Details on the results of the denaturation mechanism of α -lactalbumin by pH-dependent fluorescence spectroscopy and PARAFAC analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-245**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Detection of organophosphate ester compound using SERS substrate

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¹Kangwon National University, Korea

Organophosphate compounds have the advantages of protecting grains from pests thereby increasing the production and quality of agriculture. However, reckless use has caused environmental pollution and also used for terrorism and war because it damages to people. Therefore to detect the organophosphate compounds quickly is important. Surface-enhanced Raman scattering (SERS) is an ultrasensitive and effective detection method which is a nondestructive detection method and can provide molecular information. In this study, triethyl phosphate (TEP) and dimethyl methyl phosphonate (DMMP) which are one of the organophosphate esters, were successfully detected by SERS. Details on the result will be discussed in the presentation.

Poster Presentation : **PHYS.P-246**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Simulation Study on the anisotropic diffusion-reaction systems in condensed phases

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Efficient algorithms for anisotropic diffusion-reaction systems have been studied using lattice-based Monte Carlo simulations, which can be used to improve the applicability to complex real systems. The random walk on irregular lattices has attracted increasing attentions since it can represent numerous complicated diffusion-reaction systems such as in vivo biological reactions and percolation clusters. We find that anisotropy can be efficiently controlled by changing the probability ratio of the stay to the movement in two or three dimensional simulations. Simulation results are easily obtained and compared in anisotropic systems where theoretical predictions are absent. We confirm the accuracy of Monte Carlo methods by reproducing the theoretical predictions in isotropic diffusion-reaction systems.

Poster Presentation : **PHYS.P-247**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Unimolecular Processes of Roussin`s Red Ester for evaluation as NO-donor

Hojeong Yoon, Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Nitric oxide is a highly reactive radical and has a strong toxicity. However, it is also known to play an important role in vivo. It is synthesized in vivo and is considered to be important molecule for various immune and physiological functions. There are many substances that can produce such nitric oxide. Among them, we focus on NO-donor which can control the amount by using light. Previously known NO-donors showed photodissociation phenomena when they were exposed to UV light. Such NO-donors exist in the form bound to sulfur or transition metals. We will investigate the photodissociation dynamics of Roussin`s Red Ester (RRE), $[\text{Fe}_2(\mu\text{-RS})_2(\text{NO})_4]$, a cluster of iron and sulfur, and try to evaluate it as a NO-donor for RRE. RRE has the advantage of being able to produce stable and simple synthesis compared to other NO donors. In addition, time-resolved infrared spectroscopy is used to identify the unimolecular processes of the RRE and to evaluate how much of the RRE can actually be used. Finally, we compare stability and quantum yield with S-nitrosothiol, a well-known NO-donor.

Poster Presentation : **PHYS.P-248**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dissociation dynamics of chlorobenzene cation

HyunWook Choi, BongGyu Jeong, Seung Min Park*, Jae Kyu Song*

Department of Chemistry, Kyung Hee University, Korea

Photodissociation decay times of chlorobenzene cations ($\text{Bz}^{35}\text{Cl}^+$, $\text{Bz}^{37}\text{Cl}^+$) had been investigated by linear tandem time-of-flight mass spectrometer. Mass-selected $\text{Bz}^{35}\text{Cl}^+$, $\text{Bz}^{37}\text{Cl}^+$ were irradiated by various photons (230 to 305 nm). Photodissociation rate constant depended on the internal energy of BzCl^+ and isotope effect. Ionization energy and bond dissociation energy were calculated by Gaussian 09 program at the B3LYP / cc-pVTZ theory level of DFT method and the theoretical rate constant was calculated that the home made RRKM calculation programs.

Poster Presentation : **PHYS.P-249**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The structural and electronic properties of a $\text{Mo}_6\text{S}_3\text{I}_6$ nanowire by DFT compositional ordering

You Kyoung Chung, Weon Gyu Lee, Joonsuk Huh*

Department of Chemistry, Sungkyunkwan University, Korea

The effect of structural disorder by compositional modelling and their electronic properties of an isolated $\text{Mo}_6\text{S}_3\text{I}_6$ nanowire are investigated using density functional theory calculations. With two energy minima upon uniaxial strain relaxation, the possible structures of twelve atomic models are proposed. We find the unique atomic models of new proposed metallic conformers that are more stable than reported earlier with lattice constant $c=13.75 \text{ \AA}$. We also show the electronic band gap energy is inversely proportional to their structural stability. The quasi-1D sheets at the Fermi level from new designed semiconducting or metallic models are in good agreement with the intensity of density of states and the degree of band crossing at the Fermi level. The delocalized valence charge density differences through Mo-S bridging chains show the important role of the existence of sulfur atoms in bridging plane for intramolecular charge transport. Our studies find that the electronic band gap energy of nanowires is a quite well proportional to the integrated Mo-S bonding orbital energy due to their structural stability using crystal orbital Hamilton population (COHP) analysis. These results suggest that the compositional sites of decorative S or I atoms of an $\text{Mo}_6\text{S}_3\text{I}_6$ nanowire can be crucial for identifying the real structure of an isolated $\text{Mo}_6\text{S}_3\text{I}_6$ nanowire that is expected to be used as a wide range of key component for the applications of electronic nano-devices such as transistors, sensors, and photovoltaic devices.

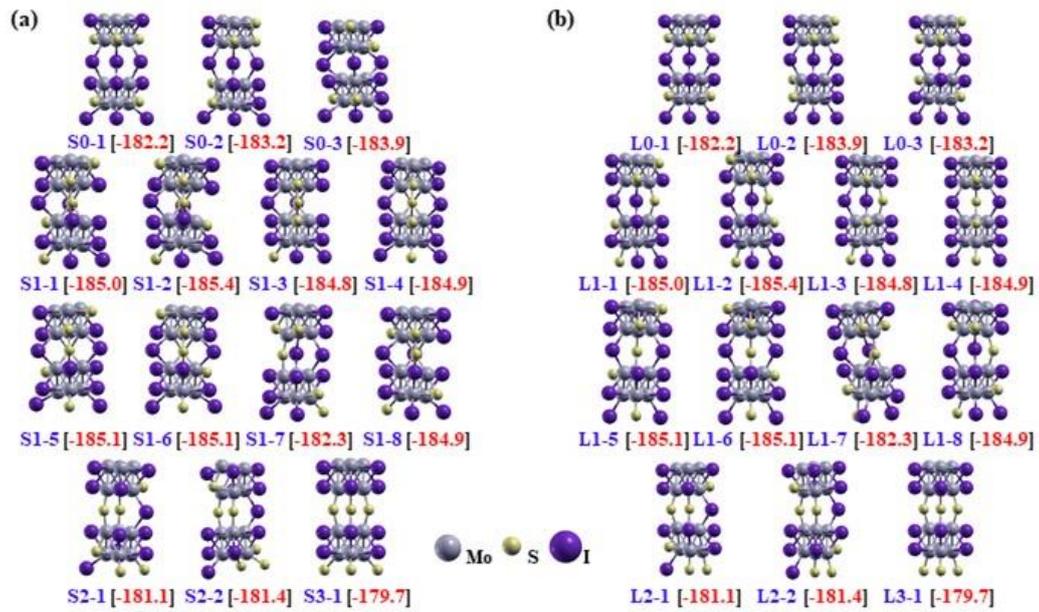


Figure. Ball and stick models of the optimized structures of various atomic $\text{Mo}_6\text{S}_3\text{I}_6$ nanowires and the total free energy (eV/unit cell) whose values are all in square brackets for (a) S-form conformers ($c=12.5$ Å), and (b) L-form conformers ($c=13.75$ Å) of $\text{Mo}_6\text{S}_3\text{I}_6$ nanowires, respectively.

Poster Presentation : **PHYS.P-250**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Measurement of Trace Atmospheric Gases with 22 GHz, 110 GHz, and 183 GHz Microwave Remote Sensing

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The ground-based microwave remote sensing is appropriate for monitoring the trace gases in the middle atmosphere continuously. The microwave radiometer detects rotational microwave emission from the polar molecules such as ozone, water vapor, chlorine oxide and so on. The microwave below 300 GHz is used for the ground-based remote sensing due to large non-resonant water vapor and oxygen continuum absorption. In this study, we will describe three ground-based microwave radiometers of 22 GHz, 110 GHz and 183 GHz at Sookmyung Women's University in Seoul. The 22 GHz radiometer is called Seoul Water vapor Radiometer (SWARA) and the 110 GHz radiometer (Stratospheric Ozone Radiometer in Seoul, SORAS) have been operated to measure the water vapor profile and ozone profile in the middle atmosphere since 2006 and 2013, respectively. The ozone and water vapor profiles in the middle atmosphere are retrieved from the integrated spectra for a few minutes or hours by the optimal estimation method. The 183 GHz microwave radiometer has been developed to detect the surface water variation and it has been operated since October 2017. It has four channels of 183.310 GHz \pm 1, 3, 4.5, 7 GHz with different bandwidth. The 183 GHz is known as fully saturated area at the ground-based remote sensing, but the variation has been detected during the winter in Seoul. In this presentation, we will show the 183 GHz brightness temperature variation with the simulation results from Radiosonde data at the same period. The retrieved ozone and water vapor profiles over Seoul from SORAS and SWARA for the last few years will be described as well. "This work is financially supported by Korea Ministry of Environment(MOE) as 「Graduate School specialized in Climate Change」."

Poster Presentation : **PHYS.P-251**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Designing Nanogadgetry: Heterojunctions of Boron Nitride and Graphene Nanoribbons for Nanoelectronic Devices

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Department of Bio-Nano Engineering, Hanyang University, Korea

Even though zigzag graphene (Z-GNR) has an excellent electrical conductivity, the lacks of an electronic bandgap that limits its potential applications in nanoscale electronics. In contrast, hexagonal boron nitride (h-BN) exhibits insulating properties with a wide band gap, and draws much attention due to its super thermal and chemical stabilities. The fusion of a zigzag graphene and a hexagonal boron nitride can form heterojunctions with remarkable electronic transport properties. In this research, we investigate the electronic transport properties of zigzag graphene/ hexagonal boron nitride heterojunction (BNCNR) with a variety of different heterojunction. We considered the initial electronic properties of graphene and h-BN. Graphene nanoribbons (GNRs) have width dependent conductance in zigzag nanoribbon and hexagonal boron nitride nanoribbons (BNNRs) have different transport properties in accordance with edge elements and hydrogen termination. We are showed that the electronic properties of heterojunction depend on the number of ribbons combined, the order of each ribbons, ribbon width, edge components and hydrogen termination in edge. The calculated results also reveal the formation and causes of the formation of conducting channels in BNCNR structures. The unique properties of our proposed BNCNR structures can be very useful for the production of nanoelectronic devices.

Poster Presentation : **PHYS.P-252**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Quantitative study of mammalian protein correlation based on chromatin interactome model

Jaehyuk Won, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

We studied analysis of mammalian cell gene expression. In mammalian cell, genes are gathering and then form transcriptional interactome. This phenomenon makes correlation of gene expression high, provides insights into transcription regulation and three-dimensional interaction are associated in occurring diseases. But, it's complicated and unknown that How can they interact and cooperatively transcribe. We designed gene specific expression model for investigating protein level correlation in chromatin interactome and use parameter that implies intricate chromatin interactions. We can analysis correlation in gene expression level much more concisely

Poster Presentation : **PHYS.P-253**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Density functional study on Carbon Nanobelts

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Many types of carbon nanorings have been proposed, but most of them have not yet been synthesized. Only the benzene ring fused with the smallest carbon nanotube [5]-C_{pp} has been successfully synthesized. Because carbon nanotubes have a planar structure of benzene, it is very difficult to overcome this strain energy and synthesize. However, Carbon nanobelts and their precursors are expected to be useful for future synthetic purposes. Because the carbon nanobelts are all benzene rings, we have been interested in the change of aromaticity. The aromatic ring current of aromatic rings is strongly related to the chemical shift, and the chemical shift of the central atom in NMR should be noticeable due to the ring current. This work performed with DFT calculations and examined the structure, magnetic properties and electrical structure of several previously proposed nanobelts. Anisotropy of the Induced Current Density (AICD) and Nucleus-Independent Chemical Shifts (NICS) techniques were used to investigate the relationship between chemical shift and ring current. 1. Povie et al., *Science*. 2017, 356, 172–1752. Yasutomo Segawa, Akiko Yagi, Hideto Ito, and Kenichiro Itami, *Org. Lett.* 2016, 18, 1430–1433

Poster Presentation : **PHYS.P-254**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Interaction of atomic and molecular hydrogen on Pd modified ZnO surfaces

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¹Department of Chemistry, Kyungpook National University, Korea

Natural zinc oxide (ZnO) contains a lot of hydrogen in the bulk and interstitial hydrogen is believed to be incorporated during crystal growth and/or by the dissociative adsorption of H₂ molecules in the atmosphere. The adsorption of hydrogen and subsequent diffusion into the bulk has been studied extensively both experimentally and theoretically. Although, natural ZnO contains a large amount of dissolved hydrogen is generally employed to place H atoms on the surface for the study of the interactions between hydrogen and ZnO. We have prepared the ZnO (0001) surface adsorbed with 0.1 ~ 10 monolayers of Pd to induce the dissociation of H₂ molecules. We will present the effect of Pd on the dissociation of H₂ molecules on the Pd/ZnO surface and subsequent diffusion into the ZnO bulk.

Poster Presentation : **PHYS.P-255**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Controllable Physical Properties of Self-doped Colloidal Quantum Dots by Alternating their Doping Density

Yunchang Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

Colloidal quantum dots have been of great interest as materials for optoelectronic devices and quantum computing, in the view of their high quantum yield in photoluminescence and tunable semiconductor properties. Among those properties, steady-state intraband transitions, arise in nanocrystals doped with the excess electron, have been spotlighted as promising materials for mid-IR application in colloidal quantum dots. The steady-state intraband transition is only observable when the electrons stay in the discrete electronic states of the conduction band, which is possible due to the absence of viable oxidation pathway arise from water or other oxidants. Due to this limitation, the number of electrons in the lowest energy state of the conduction band was challenging and rarely reported in steady-state. Here, we present the physical properties of singly occupied and doubly occupied colloidal quantum dots, which is tunable by synthesis and post-synthesis. First, absorption of the mercury chalcogenide nanocrystals can be controlled according to the size of the quantum dots at 3-10 μm , with the corresponding magnetic properties depending on the number of electrons in the conduction band. Second, we demonstrate that nanocrystals with the singly occupied quantum state (SOQS) have fascinating properties such as superparamagnetism. This novel properties make the CQDs promising candidate for the new-generation device, such as spintronics and quantum computing.

Poster Presentation : **PHYS.P-256**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Fluorescence sensor for nitroaromatic compounds based on excited-state intramolecular proton transfer

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2-(Benzothiazol-2-yl)pyren-1-ol (P3-NS) was synthesized and its photophysical and photochemical properties were studied. In nonpolar or weakly polar solvents, P3-NS undergoes excited-state intramolecular proton transfer (ESIPT) reaction upon electronic excitation. By contrast, P3-NS is deprotonated in highly polar solvents and its anionic form (P3-NS⁻) shows strong fluorescence. ESIPT reaction of P3-NS is found to take place on a few hundred femtosecond timescales. Fluorescence quenching by the ESIPT reaction of P3-NS results from intersystem crossing at conical intersection between S₁ and T₂ states. In addition, the fluorescence of P3-NS⁻ in acetonitrile is quenched by nitroaromatic compounds. The static quenching is caused by protonation of P3-NS⁻ by acidic nitroaromatic compounds and the dynamic quenching occurs by the photoinduced electron transfer from P3-NS⁻ to electron-deficient nitroaromatic compounds.

Poster Presentation : **PHYS.P-257**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational study of the role of surface water in cold denaturation.

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Stability of globular proteins has a very interesting tendency upon temperature changes. Generally, a protein forms a stable native structure near room temperature, but when the temperature increase or decrease, its native structure becomes unstable. Disruption of the native structure at low temperature is called “Cold denaturation”. It was known that cold denaturation phenomenon is caused by weakening of hydrophobic interaction as temperature decreases. In this study, we performed fully atomistic molecular dynamics simulations of a small globular protein 1DV0 as a target system. To solve thermophilic problem of empirical protein force fields, we tuned intramolecular van der Waals (vdW) parameters of hydrophobic carbon atoms, thereby improving thermal stability curve and thermodynamic parameters upon unfolding. In particular, we report free energy difference between surface water near hydrophobic residues and bulk water at cold and heat denatured state to investigate the role of surface water around hydrophobic residues when protein denaturation occurs.

Poster Presentation : **PHYS.P-258**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Conformational and dynamical behavior of collapsed polymer

Gyunam Park, Sanggeun Song, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

Most of polymers in living cells has collapsed conformation because proteins in cells make high concentration condition. Therefore, studying conformational and dynamical behavior of collapsed polymer is important for understanding biological polymer. Collapsed polymer shows multimodal radial distribution function of end-to-end distance, which means that polymer develops shell feature of beads. Contrary to expectation that higher attraction force between beads makes dynamics of polymer faster, we find that first passage time between two end beads and relaxation time become slow. and first passage time and relaxation time shows dynamical activity of polymer. we propose that shell feature of beads disturb finding end monomer each other by crowding effect.

Poster Presentation : **PHYS.P-259**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Excited State Intramolecular Double Proton Transfer Dynamics of [2,2'-bipyridyl]-3,3'-diol

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

Excited-state intramolecular proton transfer (ESIPT) is one of the most important topics in chemistry and biology. [2,2'-bipyridyl]-3,3'-diol, a good model for researching ESIPT, has two symmetric points where proton transfer can occur. Double proton transfer process of this molecule is known to be able to occur via concerted and sequential pathways. Pump-probe spectroscopy using up-conversion technique is conducted on [2,2'-bipyridyl]-3,3'-diol in cyclohexane. Time-resolved fluorescence (TF) at 450 nm, 485 nm and 580 nm is obtained at the pump wavelength of 375 nm and time resolution of 50 fs. Through the Fourier transform of TF signals, coherent nuclear wave packet oscillation in 300 cm^{-1} (strong) and 190 cm^{-1} (moderate) were observed at all detection wavelengths. These vibrational modes may be related to the proton transfer dynamics driven by skeletal motions, and theoretical investigations regarding these vibrational modes will be presented.

Poster Presentation : **PHYS.P-260**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Morphology analysis of bacterial clusters attached to column media

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The adsorption mechanism of colloidal particles such bacteria could be utilized in the many applications, including: wastewater treatment, remediation of contaminant and, risk assessment of hazardous materials. This research was conducted to analyze the morphology of bacterial clusters considering the physico-chemical properties through the experimental approaches. We selected two model bacteria as soil microbes, which is found in the soil environment. According to the previous literature, the adhesive interaction was calculated based on assumption that colloidal surfaces are homogeneous. However, the asperity of the colloid surfaces is needed to systemically interpret the interactions since there exists in real. In this study, we verified the nanoscale roughness on the bacteria using an atomic force microscope and fluorescence microscope, and compared with the interaction energy based on the Extended-DLVO theory. Results revealed that the selected bacteria have the nanoscale roughness on the surfaces unlike usual substrate (e.g., silica surface). Still, we expect that systematic conditions are needed because the bacteria have the variability with solution chemistry (e.g., ionic strength, ionic valence etc.). This research was supported by the Korea Energy and Mineral Resources Engineering Program (KEMREP).

Poster Presentation : **PHYS.P-261**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Pulse modulated Spectroscopy of NaYF₄:Yb³⁺, Er³⁺ Upconversion Phosphor

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¹Department of Bionano Chemistry, Kookmin University, Korea

Upconversion lanthanide phosphors have great potential for use in a variety of applications such as nanomedicine, solid state 3D displays, nanoscale temperature measurement and solar cell technology. The way to obtain various emission colors through synthesis is well known in previous studies, but it difficult to display certain colors. To overcome this problem, Xiaogang Liu and fellow researchers have announced a study to control the emission color of the by controlling the laser pulse width. However, the mechanism of the red emission of NaYF₄:Yb³⁺, Er³⁺, including 2, 3 and multi-photon processes, is under discussion. This study shows the red emission mechanism of NaYF₄:Yb³⁺, Er³⁺ through the modulated laser.

Poster Presentation : **PHYS.P-262**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Plasmon enhanced NaYF₄: Yb, Er upconversion films using pulsed laser deposition

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¹Department of Chemistry, Kookmin University, Korea

Some rare earth metals have a feature that has an optical phenomenon called upconversion (UC). This phenomenon occurs when two or more photons are absorbed in the excited state and emit light at a higher energy than the incident light. Using these properties, it has been used in solar cells, displays and the development of lasers laser. Recently, upconversion nano particles are increasingly applied to bio-imaging. In addition, UC materials have been used in the field of security, information, and anti-counterfeiting by producing films with patterns. However, the UC process of lanthanide series has the lowest quantum efficiency of less than 5%. Therefore, a high power light source is required to obtain information from a UC application. In order to overcome this problem, a UC thin film with a pattern was fabricated by pulse laser deposition in previous research. UC films annealed by exposure to high temperatures to improve crystallinity, and defect sites were removed to improve efficiency. However, when the substrate is thin or cannot be annealed at high temperature, there is a problem in that the film is damaged and information is deformed. In this study, we tried to increase the luminescence intensity of the upconversion material by using the plasmon effect of the noble metal, and the film was formed on the substrate by the pulsed laser deposition method. The thickness of the layer was adjusted so that the emission wavelength of the UC and the plasmon band of the noble metal were resonant. The structure of the fabricated film has various structures such as a noble metal layer is below and a sandwich structure in which a noble metal layer and an upconversion layer are intersected with each other. As a result, it was confirmed that the luminous efficiency of UC was increased in a film having a noble metal layer, and the difference between a general film and a noble metal added film was analyzed through time-resolved luminescence analysis

Poster Presentation : **PHYS.P-263**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Binary Self-Assembled Monolayer on Au(111) Derived from Alkanethiol and Adamantanethiol

Young Ji Son, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Binary self-assembled monolayers (SAMs) prepared by the spontaneous adsorption of thiols with a different backbone structure can control their respective ratio, surface morphology, and degree of phase segregation, which are very important for biological technology such as biosensors, protein immobilization and prohibition. We examined the surface structures and adsorption behaviors of self-assembled monolayers (SAMs) formed from adamantanethiol (ADT) and alkanethiol (AT) with different chain lengths using co-adsorption or displacement methods by scanning tunneling microscopy (STM) and cyclic voltammetry (CV). It was found that the phase segregation of binary SAMs prepared by co-adsorption of ADT and AT was dominantly appeared when alkyl chain length of AT increased. In addition, binary SAMs with different molar ratio were formed via the displacement of pre-covered ADT SAMs by AT as a function of displacement time.

Poster Presentation : **PHYS.P-264**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Non-classical Theoretical Investigation of the Role of the Nuclear Envelope in Living Cells

Jingyu Kang, Ji-Hyun Kim^{*}, Jaeyoung Sung^{*}

Department of Chemistry, Chung-Ang University, Korea

There are two types of cells: *eukaryotes*, which have a nuclear envelope inside the body, and *prokaryotes*, which do not. This distinction between eukaryotes and prokaryotes is well known, yet the role of the nuclear envelope is not well understood. Of the numerous effects caused by the existence of the nuclear envelope, several studies investigated the noise of the mRNA copy number compared to the mean mRNA copy number. However, these theoretical studies are limited to only considering the classical chemical kinetics, that is, Pauli's master equation, utilizing only the differential equation to determine mRNA number. The classical chemical kinetics itself is limited in that it can only provide a qualitative analysis of experiments. Therefore, in the current research, we take advantage of a non-classical chemical kinetics for the quantitative analysis of mRNA copy number fluctuation as a function of mean mRNA number. Making use of our own theoretical tools, we can further study the dynamics inside the nuclear envelope by analyzing the auto-correlation function and the cross-correlation function between mRNA in the nucleus and mRNA in the cytoplasm, an unprecedented achievement under the classical theory.

Poster Presentation : **PHYS.P-265**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Adsorption structures of N-containing aromatic molecule pyrazine on Ge(100)

Jeonghui Choi, Do hwan Kim*

Department of Chemical Education, Chonbuk National University, Korea

The adsorption reaction of pyrazine on Ge(100) was studied using density functional theory (DFT) calculations. These calculations predicted that pyrazine, N-containing aromatic organic molecule, would initially adsorb on Ge surface through N-dative bonding. Bidentate structure bridging two adjacent dimer rows are the most stable among all the tested structures. Single dative bonding with N-Ge linkage was also stable, which can be compared with experimental STM results. Simulated STM images explained the change in electron charge density that would occur upon the adsorption of pyrazine in various adsorption structures.

Poster Presentation : **PHYS.P-266**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Molecular dynamics study on phase transition of imidazolium-based organic ionic plastic crystal

JungBin Park, Bong June Sung*

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Organic ionic plastic crystal (OIPC) is a unique crystal phase that exhibits rotational disorder while ions maintain a long-range ordered crystalline lattice structure. Plastic crystal materials have attracted much attention as an electrolyte because the rotational disorder accelerates the diffusion of mobile ions, such as lithium cation. However, only a small number of combinations of cation and anion have OIPC phase because rotational motion is restricted by molecular shape of ions and the lattice symmetry. Therefore, identifying the ion pair that may OIPC phase and understanding the fundamental dynamics of OIPC are important in designing novel materials toward improved electrochemical performances. In this work, we perform molecular dynamics simulations to investigate the physical origin of OIPC phase systematically and phase transitions of three imidazolium-based ionic crystal; 1) 1-methyl-3-methylimidazolium dicyanamide ([mmim][tfsi]), 2) 1-methyl-3-methylimidazolium chloride ([mmim][cl]), and 3) 1-butyl-3-methylimidazolium chloride ([bmim][cl]). A series of simulations are performed by employing each perfect crystalline experimental structure. We find solid-solid phase transitions in [bmim][cl] and [mmim][tfsi] crystal, whereas [mmim][cl] crystal undergoes only solid-liquid transition at melting temperature (420K) without any solid-solid transition. On the other hand, molecular rotation along axis of butyl group brings a rotator-solid phase to [bmim][cl] under its melting temperature (325K). In case of [mmim][tfsi], the crystal shows not only a rotator-solid phase, but also a diffusive-solid phase where hopping diffusion occurs within lattice structure.

Poster Presentation : **PHYS.P-267**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dynamics of Single-Molecular Dichotomic Process with a Time-Dependent Hidden Environmental Variable

Hunki Lee, Ji-Hyun Kim*, Jaeyoung Sung*

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The function of transcription factors is to regulate – turn on and off – genes to make sure that they are expressed at the right time and in the right amount throughout the life of the cell. However, previous studies for the feedback have used simplified the process from binding and unbinding process of DNA polymerase to a promoter to transcription process resulting details of dynamical and quantitative information are ignored. In this study, we consider the binding and unbinding process of DNA polymerase to predict the dynamical behavior of the system more precisely. A model is proposed for a rate process through a bottleneck with Ornstein-Uhlenbeck process as an reference model.

Poster Presentation : **PHYS.P-268**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The effects of Nanoparticles on the Glass Transition Temperature of Thin Polymer Films

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The glass transition temperature (T_g) is one of the most important properties for processing thin polymer films. A recent experiment found that the T_g of the thin polymer film was decreased by 65 degrees by adding and changing a spatial distribution of NPs. [Nano. Lett. 2008, 8, 2271-2276] Our previous simulation study [Soft Matt. 2017, 13, 5897-5904] found that NPs were distributed either at center or in the surface region in polymer film depending on the size and the interaction type of NPs. However, it still remains elusive how the spatial distribution of NPs affects the T_g of the film. In this research, we use molecular dynamic (MD) simulations and generic coarse-grained models for both a polymer and NPs to investigate the relationship between the spatial distribution of the NPs and T_g of the thin polymer film. Small (large) NPs are mainly located at a surface (center) layer of the film and an attractive (non-attractive) interaction makes NPs move to a center (surface) region of the film. The mobility of polymers is increased (decreases) as one makes the interaction more attractive (non-attractive) NPs. The mobility of polymers at the film center is affected more significantly than polymers at the surface. Such effects of NPs on the polymer mobility lead to a change in T_g .

Poster Presentation : **PHYS.P-269**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Atomic and electronic structure of Acetaldehyde on Ge(100)

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The carbonyl(C=O) group may be a good precursor for tethering large molecules to the surface for use in device applications where the transport of charge through the molecule is important. Especially we concerned the acetaldehyde which is the tautomer of vinyl alcohol. Chemisorption of acetaldehyde with Ge(100) surface has been investigated using density functional theory (DFT) calculations. The calculations show that the carbonyl(C=O) group can undergo cycloaddition onto the Ge dimer on the Ge(100) surface. The C=O [2+2] cycloaddition product is more favorable structure than other adsorption reactions (C-H dissociative reaction and Ene-reaction). Thus the surface adsorption of acetaldehyde on Ge(100) will form Ge-O-C-Ge bonding. The effect of bias voltages on the electronic charge density has been also investigated within the Tersoff-Hamann scheme. From the results of our DFT calculations, we conclude that the adsorption of acetaldehyde on Ge(100) proceeds in similar reaction result to other simple system of carbonyl compound (formaldehyde, acetone) on Si, differs from the reactions of acetaldehyde on Si(001) and on Ge surface.

Poster Presentation : **PHYS.P-270**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The Mid-IR Electronic Transition of Self-doped Colloidal Quantum Dot

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Department of Chemistry, Korea University, Korea

The colloidal quantum dots (CQDs) have been actively studied for the last three decades. Recently, there was a great advance in the study of the intraband transition. The first steady state mid-IR intraband transition was reported by Jeong et al. in 2014 and this innovation suggested a new direction of CQDs. In this poster, I will present the mid-IR photoluminescence of the intraband transition from the self-doped Ag₂Se and CdHgSe nanocrystals. The silver chalcogenide alleviates the apprehension about the toxicity of the mid-infrared intraband transition nanocrystals and renders a new possibility of non-toxic intraband CQDs. The Ag₂Se nanocrystals had been regarded as a nanomaterial having a bandgap transition in the mid-IR region. The spectroelectrochemistry and mid-IR emission results of Ag₂Se, however, proved the mid-IR electronic transition is originated from the intraband transition rather than the bandgap transition. The mid-infrared emission was measured by using the home-made mid-infrared emission spectrometer. Surprisingly, the intraband transition can be generated by cation exchange method. The CdHgSe alloy synthesis has shown the interesting optical property that the major electronic transition shifts from the visible to mid-IR LSPRs by increasing the portion of mercury in the nanocrystals. The carrier density of the CdHgSe has increased to semi-metal as electronic transition shift by self-doping property of intraband nanocrystal. The photosensitivity and the PL results were obtained to determine the stoichiometric effect of sample characteristics.

Poster Presentation : **PHYS.P-271**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Accurate measurements and reliable prediction of ΔE_{ST} of TADF molecules

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Thermally activated delayed fluorescence (TADF) is an important process for efficient harvesting of triplet excitons in small molecule organic light-emitting diodes (OLEDs). Accurate measurements of the energy gap between singlet and triplet excited state (ΔE_{ST}) and reliable prediction of ΔE_{ST} by quantum chemical calculations are essential to characterize and design TADF molecules to achieve almost 100% internal quantum efficiency. In this work, we developed a frequency and time-resolved photoluminescence spectroscopy at 77 K to measure fluorescence and phosphorescence spectra separately and determine ΔE_{ST} of TADF molecules. In addition, time-dependent density functional theory (TD-DFT) method with gap-tuned range-separated DFT functionals was employed to predict ΔE_{ST} of TADF molecules reliably.

Poster Presentation : **PHYS.P-272**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Crystallographic analysis of the pi-pi interactions in the crystal packing of selenothymidines

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4'-seleno nucleosides are 3rd generation of nucleosides which has been developed for the anti-viral agent. The crystal structure of deoxy 4'-selenothymidine has been determined by the direct method. In order to show how the differences in the fine molecular structures of 4'-seleno nucleosides represent the differences in intermolecular interactions and how crystal packing differs therefrom, we compared the crystal packing of three 4'-seleno thymidines for the influence of pi-pi interactions in crystal packing. 4'-selenothymidine is tangled up with lots of hydrogen bonding. Deoxy 4'-selenothymidine is stacked stably like DNA with strong and regular pi stacking. And dehydro deoxy 4'-selenothymidine is packed with T-shaped pi interaction with parallel displaced pi interactions. These results indicate that the pi-interactions are very important determinant in crystal packing and intermolecular interactions.

Poster Presentation : **PHYS.P-273**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Induced circular dichroism of jet-cooled phenol complex with 1-amino-2-propanol

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Molecular interactions between achiral and chiral molecules give rise to circular dichroism within the absorption region of the achiral molecule, which is called induced circular dichroism (ICD). ICD spectroscopy has extensively been used to probe the interactions between host and guest molecules in solution. However, ICD spectra measured in solution exhibit only the averaged ICD values of all conformational isomers. To obtain the conformation-specific ICD values, we need to apply ICD spectroscopy to molecular complexes in the isolated gas phase. Here, we obtained the first ICD spectra of jet-cooled phenol (PhOH) complexes with (-)-1-amino-2-propanol (AP) using resonant two-photon ionization (R2PI) CD spectroscopy. The R2PI spectra of PhOH-AP exhibit well-resolved vibronic bands of three different conformers, which have different ICD signs and magnitudes. These differences in the ICD values were explained by the different geometrical asymmetries of the PhOH moieties in the conformers and their different strengths of the electronic coupling between PhOH and AP.

Poster Presentation : **PHYS.P-274**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Morphological Changes of Binary and Ternary Systems during Solvent Evaporation: Coarse-Grained Molecular Simulations

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Organic Photovoltaics (OPVs) are a promising device for harvesting solar energy, but they still suffer from critical problems such as phase separation and degradation in efficiency, which hampers their commercial applications. Researchers are looking for various ways to solve the problems by developing new materials or by introducing several components into the device. Recently, Go group [1] reported that increasing the number of OPVs components can not only enhance the OPVs efficiency but also stabilize its long-time morphology. So, in this study, we made binary and ternary systems through coarse grain molecular simulations and compared the morphology of the multi-component systems. At this time, poly(3-hexylthiophene) (P3HT) was used for the donor and phenyl-C₆₁-butyric acid methyl ester (PC61BM) and [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC71BM) were used for the acceptor because these are widely used. Through these systems, we investigated the molecular mechanism of the effects of OPVs components on the morphological changes of the OPVs system. In the end, we observed that the ternary system exceeds the binary systems in the long-time stability of the OPVs device.[1] Nam, M.; Cha, M.; Lee, H. H.; Hur, K.; Lee, K.-T.; Yoo, J.; Ki Han, Il; Kwon, S. J.; Ko, D.-H. Nat Comms 2017, 8, 1–10.

Poster Presentation : **PHYS.P-275**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Molecular dynamics simulations for thin films of the ring and linear polymer blends

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The topology of ring polymer leads to an interesting different diffusion mechanism: ring polymers exhibit amoeba-like motion while linear polymers exhibit reptation motion. Also, the glass transition temperature (T_g) of ring polymers may be different from that of linear polymers. For example, low molecular weight ring poly(dimethylsiloxane) shows higher by 20K than linear counterparts []. Therefore, blending ring and linear polymers is expected to control, viscosity and fragility of the material especially as in the form of a film. However, few studies are carried out to understand the dynamics and glass transition of ring and linear polymer mixtures, especially in polymer films. In this study, we perform molecular dynamics simulations and examine the effects of ring polymers on free-standing ring-linear polymer blend thin films by varying the fraction of linear polymers. For every, ring exhibits faster translational and rotational motions than linear polymers. The non-Gaussian parameter of ring polymers is also slightly lower than the linear polymers. In the future study, we will investigate how those properties would change with the film thickness and ring polymer composition.

Poster Presentation : **PHYS.P-276**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

An Investigation on the photosensitization behavior and energy transfer dynamics of dendritic Ir-complex decorated with carbazole units through transient absorption spectroscopy and singular value decomposition analysis

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Department of Advanced Materials Chemistry, Korea University, Korea

In order to investigate the light-energy harvesting mechanism, a series of dendrimers with a heteroleptic iridium(III) complex core, [Ir(dmb)₂(pic-Cz_n)] (G_n: n = 1, 2, and 3), with 2,6-difluoro-3-(4-methylpyridin-2-yl)benzotrile (dmb) as the cyclometallating ligand and 3-hydroxypicolinate (pic) as the ancillary ligand, connected to carbazole-based dendrons (Cz_n: n = 2, 4, and 8) was synthesized. The Ir centred complex [Ir(dmb)₂(pic-OCH₃), G₀] shows a blue emission at ³MLCT phosphorescence. This phosphorescence was enhanced with increasing generations due to the increase in the total absorbance of the Cz-dendron. The light-harvesting efficiencies determined by various methods were approximately 160 (G₁), 220 (G₂), and 330% (G₃). The energy transfer efficiencies for G₁–G₃ from the peripheral Cz-dendron to the Ir-core complex were above 97%, determined using the reduction in the lifetime of the excited ¹Cz*-dendrons. G₁–G₃ showed a transient absorption (TA) band at 600 nm, which was attributed to the S_n←S₁ transition of the Cz-dendrons. The fast decay of these TA bands was consistent with the fast emission decay times. The time-resolved TA band correlated with the core Ir-complex was observed at 500 nm, though it overlapped and interfered with the intense TA band of the Cz-dendrons. Therefore, we attempted a global analysis by singular value decomposition (SVD). The determination of the absorption spectra of the individual species participating in the energy transfer process by SVD analysis can distinguish between different mechanistic models. The analysed rate constants were consistent with the results determined by the emission decays.

Poster Presentation : **PHYS.P-277**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Inter-Ligand Energy Transfer (ILET)-based Excited state dynamics of photoactive heteroleptic iridium complexes

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In order to understand the causes of the emission shape and colour changes of heteroleptic Ir³⁺ complexes containing 2-(2,4-difluorophenyl)pyridine (dfppy) as the main ligands, we introduced two types of ancillary ligands: (1) non-luminescent ancillary ligands, namely tetrakis(pyrazolyl)borate (bor) and picolate (pic), which were employed for the preparation of Ir(dfppy)₂(bor) and Ir(dfppy)₂(pic), respectively, and (2) luminescent ancillary ligands, namely 1,10-phenanthroline (phen), bipyridine (bpy), and 2,3-dipyridylpyrazine (dpp), which were employed for the preparation of Ir(dfppy)₂(phen), Ir(dfppy)₂(bpy), and Ir(dfppy)₂(dpp), respectively. The anomalous rigidochromism was attributed to an interligand energy transfer (ILET), and showed a strong temperature dependence. The ILET occurs from dfppy to the other ligands lying in lower energy states. The ILET dynamics were probed directly using femtosecond transient absorption (TA) spectroscopy after the excitation of dfppy.

Poster Presentation : **PHYS.P-278**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Cationic effect on KIE and equilibria of the ESPT reaction of C183 in aqueous solutions

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Physical properties and hydrogen network of water in aqueous ionic solutions differ greatly from those of neat water due to dissolved ions. In this work, the ionic effects on the excited-state proton transfer (ESPT) reaction of Coumarin 183 (C183) in aqueous ionic solutions are studied in terms of pKa, pKa*, activation energies (Ea), and kinetic isotope effect (KIE). The acid dissociation constants of C183 on the ground state (pKa) and excited states (pKa*) are determined by steady-state emission and UV-visible absorption spectroscopy. The activation energies and KIE for the ESPT reaction of C183 in each ionic solution are directly obtained by using time-resolved fluorescence spectroscopy. It is found that pKa, pKa*, Ea, and KIE values for the ESPT reaction of C183 are significantly influenced by cations (more accurately by the charge density of cations). Especially, the secondary KIE is more vulnerable to the effect of cations compared to the primary KIE. Furthermore, the effects of cations on the equilibria (pKa, pKa*) and kinetic (Ea, KIE) parameters of C183 are well explained by the free-energy reactivity relation. Our current results give valuable insight to understanding the fundamental ionic effect on the equilibria and kinetics of ESPT reaction in aqueous ionic solutions.

Poster Presentation : **PHYS.P-279**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Detailed Investigation of Photoinduced Electron Transfer Dynamics in a BODIPY-*ortho*-Carborane Dyad

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We report the results of photoinduced electron transfer (PET) in a novel dyad, in which a boron dipyrromethene (BODIPY) dye is covalently linked to *o*-carborane (***o*-Cb**). In this dyad, BODIPY and ***o*-Cb** act as electron donor and acceptor, respectively. PET dynamics were investigated using a femtosecond time-resolved transient absorption spectroscopic method. The free energy dependence of PET in the S1 and S2 states was examined on the basis of Marcus theory. PET in the S1 state occurs in the Marcus normal region. Rates are strongly influenced by the driving force ($-\Delta G$), which is controlled by solvent polarity; thus, PET in the S1 state is faster in polar solvents than in nonpolar ones. However, PET does not occur from the higher energy S2 state despite large endothermic ΔG values, because deactivation via internal conversion is much faster than PET.

Poster Presentation : **PHYS.P-280**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Time-resolved studies on singlet exciton fission in perylenediimide-derivatives

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Singlet exciton fission (SEF) is a spin-allowed process in which two triplet excitons are produced from one singlet exciton when the energy of singlet exciton is greater than twice of the energy of triplet exciton. SEF is a fundamentally interesting phenomenon and has attracted great attention for maximizing the external quantum efficiency in solar cells by overcoming the Shockley-Queisser limit. For this purpose, pentacene- and tetracene-derivatives have been extensively studied. In this work, we investigated the SEF process in two perylenediimide-derivatives in films and solutions by using UV-vis absorption, emission, and time-resolved fluorescence spectroscopy in conjunction with the density functional theory (DFT) calculations.

Poster Presentation : **PHYS.P-281**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Intramolecular charge transfer studied by time-resolved Raman spectroscopy

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The intramolecular charge transfer (ICT) state formed by charge separation between the electron donor and acceptor groups upon photo-excitation was explored for fluorescent dye DCM and LD 688 in polar solvent (DMSO). Both dyes show the ICT process of ~1 ps followed by ~5 ps vibrational relaxation. Two distinct Raman spectra for the locally-excited and charge-transferred conformers in the excited state were observed from femtosecond stimulated Raman spectroscopy. Based on TDDFT simulations, a “twisted” molecular geometry with rotated dimethylamino group is proposed for the ICT state. The ICT state of LD 688 was also evidenced by the blue-shift of $\nu_{\text{ring}}(\text{C}=\text{C})$ mode ($1485 \rightarrow 1505 \text{ cm}^{-1}$) and by two nitrile bands. The development of time-resolved impulsive stimulated Raman spectroscopy will be introduced, where the coherent nuclear wave-packet motions excited impulsively by Raman pump is detected by Raman probe. The frequency-domain vibrational spectra were obtained by using Fourier-transform of the temporal response of the probe signal, where the vibrational spectrum of the sample can be obtained with much improved signal-to-noise ratio in the low frequency region of

Poster Presentation : **PHYS.P-282**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaluating the origin of aggregation-induced emission in *N,N*-diphenyl-1-naphthylamine-*o*-carborane derivatives: Its excitation spectroscopic and synchronous fluorescence spectroscopic investigation

So-Yoen Kim, Dae won Cho^{*}, Sang Ook Kang, Ho-Jin Son^{*}

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We have synthesised mono-(**NpCb**) and bis-[(*N,N*-phenyl-1-naphthylamino)benzo]-*o*-caboranes (**NpCbNp**), which show anomalously intense aggregation-induced emission (AIE) at long wavelengths and monomer emission at short wavelengths. The actual concentration of the aggregator in intense AIE is very low, so absorption spectroscopy is unsuitable for detecting small changes in the absorbance. Hence, to understand the aggregation pattern, we employ excitation spectroscopy, since this method has excellent sensitivity in compliance with the emission intensity. Moreover, we carried out synchronous fluorescence spectroscopic measurements to confirm that the aggregator is different from the monomeric species. The excitation spectrum shows distinguishable differences between the AIE and the normal emission. For the triad **NpCbNp**, the excitation spectrum for the AIE is located at a shorter wavelength than that for the monomeric emission spectrum, which means that the AIE is attributed to the H-type aggregator. On the other hand, for the dyad **NpCb**, the excitation spectrum for the AIE is observed at an identical wavelength as that for the monomeric species, which indicates that the aggregator is of the oblique type.

Poster Presentation : **PHYS.P-283**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Frequency Spectrum of Biological Noise: A Exploration of Reaction Dynamics in Living Cells

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Even in the steady-state, the number of biomolecules in living cells fluctuates dynamically; and the frequency spectrum of this chemical fluctuation carries valuable information about the mechanism and the dynamics of the intracellular reactions creating these biomolecules. Although recent advances in single-cell experimental techniques enable the direct monitoring of the time-traces of the biological noise in each cell, the development of the theoretical tools needed to extract the information encoded in the stochastic dynamics of intracellular chemical fluctuation is still in its adolescence. Here, we present a simple and general equation that relates the power-spectrum of the product number fluctuation to the product lifetime and the reaction dynamics of the product creation process. By analyzing the time traces of the protein copy number using this theory, we can extract the power spectrum of the mRNA number, which cannot be directly measured by currently available experimental techniques. From the power spectrum of the mRNA number, we can further extract quantitative information about the transcriptional regulation dynamics. Our power spectrum analysis of gene expression noise is demonstrated for the gene network model of luciferase expression under the control of the Bmal 1a promoter in mouse fibroblast cells. Additionally, we investigate how the non-Poisson reaction dynamics and the cell-to-cell heterogeneity in transcription and translation affect the power-spectra of the mRNA and protein number.

Poster Presentation : **PHYS.P-284**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Exploiting the Cage Strain of C₂₀: MP2 and Density Functional Calculations

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By using the DFT and MP2 calculations, we studied five cage isomers. We optimized all structures without any constraints. We analyzed the bond distances and the volume of each fullerene cage. And we compared the energy difference, the vibrational frequencies, the atomic structures, and electronic properties among them. There were three isomers on the metastable state and two isomers on the transition state. By comparing the energies and atomic structures of three metastable isomers we got the strain difference of them.

Poster Presentation : **PHYS.P-285**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Excited State interaction and Photochemical Reactivity of *bis*-aryls-*o*-carboranes

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Two different types of *bis*-aryl compounds were chosen to this end; one with di-phenyls and its fused fluorenyl and the other with two isomers of naphthyls, α - and β -forms. The ground state structures confirmed by the crystallographic measurements provided a close correlation of structure and electronic property. HOMO and LUMO energies were estimated and confirmed by cyclic voltammograms and DFT calculations, respectively. Excited states were calculated by the TD-DFT calculations and correlated with the corresponding absorption spectra to illustrate the electronic perturbation in a systematic fashion that excited states were found to be lowered in regard to the electronic perturbation. Final verification of the lowered energy was made from the measurement of the electron transfer efficiency between the well-studied Iridium based photosensitizer, Ir(ppy)₃ and two typical *bis*-aryls-*o*-carboranes, α -**Np** and **Ph** and electron transfer efficiency of α -**Np** is ten times greater than that of **Ph**.

Poster Presentation : **PHYS.P-286**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Excited state structural dynamics of copper(I) bis(phenanthroline) investigated by time-resolved electronic and vibrational spectroscopy

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Transition metal complexes often show distinct photophysical properties arising from the structural symmetries and are widely adopted in many applications including photocatalysts, solar cells, OLEDs, therapeutic agents, etc. Copper(I) diimine complexes show a tetrahedral geometry in the ground state, but Cu(I) oxidizes to Cu(II) with the subsequent structural changes in the complexes from the metal-to-ligand charge transfer (MLCT) state in the excited states. Ultrafast structural changes of diimine ligands into a so-called “flattened” square-planar-like geometry have been studied by femtosecond transient absorption and fluorescence upconversion techniques, where the dynamic effects of steric hindrance in the substituted ligands have been investigated.^{1,2} In this work, excited state dynamics and structural changes of Cu(I) bis(1,10-phenanthroline) complex have been explored by combining time-resolved electronic and vibrational spectroscopy with femtosecond time scales. The flattening dynamics of phenanthroline ligands of 260 fs often observed from the changes in the excited state absorption signals will be further verified with femtosecond stimulated Raman spectroscopy. The excited state dynamics of Cu(I) bis(1,10-phenanthroline) is somewhat complex with the intersystem crossing to the T₁ state and the internal conversion to the ground state, and thus shows a strong dependence on solvent polarity. **References** 1. J. V. Lockard, S. Kabehie, J. I. Zink, G. Smolentsev, A. Soldatov, L. X. Chen, *J. Phys. Chem. B* **114**, 14521–14527 (2010). 2. L. Hua, M. Iwamura, S. Takeuchi, T. Tahara, *Phys. Chem. Chem. Phys.* **17**, 2067–2077 (2015).

Poster Presentation : **PHYS.P-287**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Excited State Dynamics of 4-Dimethylamino-4'-nitrobiphenyl Confined in Reverse Micelles

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Intramolecular charge transfer (ICT) processes in the excited states have been of great interest in biology and chemistry due to the applications to solar energy conversion, photovoltaics, fluorescence sensing, etc. When the electron donor and acceptor groups are linked by π -conjugation inside the chromophore, a torsional relaxation involved with intramolecular charge transfer states is often found in the excited state. The biphenyl groups of 4-dimethylamino-4'-nitrobiphenyl (DNBP) are connected by a C-C single bond with the donor and acceptor groups attached to the opposite ends. DNBP shows the torsional angle of the biphenyls of ~ 40 degrees in the ground state, but the torsional dynamics in the excited states would result in planar or perpendicular geometry depending on the formation of the ICT state and solvent polarity. In this research, excited state ICT dynamics of DNBP in solutions and the reverse micelles has been investigated by time-correlated single photon counting and femtosecond transient absorption techniques. The absorption and emission spectra and the ICT dynamics of DNBP showed a strong dependence on the solvent properties like polarity and viscosity. We also found that the emission of DNBP is strongly enhanced in small reverse micelles, where the ICT dynamics of DNBP is strongly restricted due to the confined geometry of reverse micelles.

Poster Presentation : **PHYS.P-288**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Exploiting the bond structures of H₃ in C₇₀ Fullerene

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By using the hybrid DFT B3LYP/6-31G* method with and without the long-range interactions, we studied the atomic structures and electronic properties of H₃@C₇₀ fullerene. We optimized all structures without any constraints. We analyzed the bond distance of hydrogen species in each cage, the change of the volume of fullerene cages, and the electron transfer between H₃ and C₇₀ in each cage.

Poster Presentation : **PHYS.P-289**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Cold Ion Spectroscopy of Protonated Phenylalanine

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We have obtained the ultraviolet photodissociation (UVPD) spectra of protonated phenylalanine (PheH^+) complexes with water molecules ($\text{PheH}^+(\text{H}_2\text{O})_n$, $n=1-4$) using electrospray ionization quadrupole ion trap time-of-flight (ESI-QIT-TOF) mass spectrometry. The $\text{PheH}^+(\text{H}_2\text{O})_n$ were produced by trapping PheH^+ in a Paul trap at 170 K filled with water vapour. Two major photodissociation (PD) channels of PheH^+ and $\text{PheH}^+\text{-H}_2\text{O}$ generating the fragment ions of m/z 75 and m/z 120 were identified. From the IR-UV hole burning (HB) spectra of PheH^+ , we found that there are two different conformers contributing to both PD channels. Although the PD channel of m/z 75 is dominant for PheH^+ , the PD channel of m/z 120 became more dominant for $\text{PheH}^+(\text{H}_2\text{O})_n$. From the IRPD and IR ion dip spectra, we found that $\text{PheH}^+(\text{H}_2\text{O})_1$ exists as at least five different conformers in the cold QIT at $\sim 8\text{K}$. We will discuss possible reasons for the alteration of the major PD channel from m/z 75 to m/z 120 in $\text{PheH}^+(\text{H}_2\text{O})_n$.

Poster Presentation : **PHYS.P-290**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis, Characterization, and excited state dynamics of cyclometalated Ir(III)–Pt(II) and Ir(III)–Ir(III) bimetallic complexes bridged by dipyridylpyrazine

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We investigated the electrochemical and excited-state properties of 2,3-bis(2-pyridyl)pyrazine (dpp)-bridged bimetallic complexes, (L)₂Ir-dpp-PtCl [**1**, L = 2-(4',6'-difluorophenyl)pyridinato-N,C² (dfppy); **2**, L = 2-phenylpyridinato-N,C² (ppy)] and [(L)₂Ir]₂(dpp) [**3**, L = dfppy; **4**, L = ppy] compared to monometallic complexes, (L)₂Ir-dpp (**5**, L = dfppy; **6**, L = ppy) and dpp-PtCl (dpp-Pt^{II}Cl₂; **7**). The structures of **1**, **3**, **5**, and **6** showed that **1** and **3** have approximately coplanar structures of the dpp unit, while the non-coordinated pyridine ring of dpp in **5** and **6** is largely twisted with respect to the pyrazine ring. Their electrochemical and photophysical properties revealed that efficient electron-transfer processes predominated in the bimetallic systems regardless of the second metal participation. The TA study further confirmed that the planarity of the dpp had a direct correlation with the degree of nonradiative decay from the emissive iridium-based ³MLCT to the Ir d–d or Pt d–d state.

Poster Presentation : **PHYS.P-291**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Catalytic and Sensor Applications of Copper Nanoparticles-Reduced Graphene Oxide Composites.

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Graphene has been recognized as a high performance catalyst support due to its high surface area, exceptional thermal/electrical conductivity and good chemical stability. Thus many attempts have been made to prepare graphene based composites as catalytic materials in order to exploit the specific advantages of graphene. In this work, a reduced graphene oxide (rGO) based composite with copper nanoparticles (CuNPs) has been synthesized and used as a catalyst for the reduction of 4-nitrophenol by NaBH₄ and as a sensor for the electrocatalytic determination of nitrite ions (NO₂⁻). The morphology of the prepared nanocomposite was characterized using various methods including transmission electron microscopy and dispersive X-ray spectroscopy. The as-prepared CuNPs-rGO nanocomposites displayed excellent resistance against oxidation and coagulation, and successful catalytic activity towards the chemical reduction of 4-nitrophenol to 4-aminophenol by NaBH₄. In addition, the CuNPs-rGO modified glassy carbon electrode showed excellent catalytic activity toward the electro-reduction of nitrite ions, due to the presence of rGO with high specific surface area and CuNP with high electron transfer capability.

Poster Presentation : **PHYS.P-292**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Layer-by-Layer Self-Assembly of Palladium Nanoparticle-Reduced Graphene Oxide Film as an Efficient Non-Enzymatic Sensor for Glucose and Hydrogen Peroxide Detection

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An efficient non-enzymatic electrochemical sensor based on layer-by-layer (LbL) self-assembly of palladium nanoparticle (PdNPs) and reduced graphene oxide (rGO) nanosheets was developed for both glucose and H₂O₂ detection. The (PdNPs/rGO)_n film was synthesized through the *ex situ* strategy, where 4-dimethylaminopyridine (DMAP)-stabilized Pd nanoparticles were prepared from the aqueous phase reduction of Na₂PdCl₄ using NaBH₄ in the presence of DMAP. The resultant positively charged DMAP-stabilized PdNPs as electrocatalysts in conjunction with negatively charged rGO nanosheets as support materials were utilized as nanobuilding blocks for sequential LbL self-assembly of (PdNPs/rGO)_n (n=1~4) film on an indium tin oxide (ITO) electrode. The successful growth of each multilayer was monitored by the gradual increase of absorbance upon increasing the number of bilayers in UV-vis spectra. The uniform multilayer formation with well-dispersion of AuNPs after each LbL assembly was confirmed by scanning electron microscopy and dispersive X-ray spectroscopy. Benefiting from the LbL self-assembly, the as-prepared glucose and H₂O₂ sensor displays excellent performance with high sensitivity, selectivity, and long term stability.

Poster Presentation : **PHYS.P-293**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Facile Synthesis of Gold Nanoparticles Coated with Graphitic Carbon Layers by Pulsed Laser Ablation in Liquid(PLAL)

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Recently, Ni nanoparticles(NPs) encapsulated by graphitic carbon(GC) and nitrogen-doped graphitic carbon(NdGC) have been synthesized in hexane and acetonitrile, respectively, by pulsed laser ablation in liquid(PLAL). In this study, Au NPs containing GC and NdGC (Au@GC and Au@NdGC) shells were prepared by pulsed laser ablation in Hexane and Acetonitrile, respectively. Au NPs without carbon shells were synthesized by PLA in methanol and deionized water to compare with both Au@GC and Au@NdGC,. The structure, composition and morphology of the Au NPs prepared in this study was characterized by UV-Visible spectroscopy, photoluminescence, Micro-Raman, XPS, SEM and HRTEM. We found that GC layers were not formed onto the Au NPs whose was larger than size 100 nm. Moreover, we obtained the Au NPs less 100 nm by dissolving the large Au NPs having no GC layers with strong acid. We hope that this contribute to various potential applications in biomaterials, surface enhanced Raman spectroscopy and catalysts.

Poster Presentation : **PHYS.P-294**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

IR Induced Isomerization of Invisible Isomers using Nanosecond Laser Spectroscopy

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Conformational structures of biomolecules play crucial roles in many physical and chemical processes, including molecular recognition and hydrogen bonding in the biological systems. Thus, investigating the conformational landscapes of small biomolecules is one of the interesting research topics in physical chemistry. Experimental and theoretical studies on the jet-cooled target molecules were carried out to investigate their structural and physical properties in the gas phase. In particular, ortho-substituted phenols, such as 2-aminophenol (2-AP), 2-hydroxyformanilide (2-HFA), and 2-acetaminophenol (2-AAP) were cooled down in the molecular beam by the supersonic jet expansion and investigated with the combination of quantum chemistry calculations and various laser spectroscopic techniques, such as, mass-selected one-color resonance two-photon ionization (R2PI), UV-UV hole-burning (UV-UV HB), and IR-dip spectroscopy. The ortho-substituted phenols, having a strong intramolecular hydrogen bonding, are usually short-lived (faster than ps) such that the conformers are rarely observed in the spectrum obtained by nanosecond laser systems. Thus, we have only observed the conformers of ortho-substituted phenols without having a strong intramolecular hydrogen bond. In this work, we have observed the spectral features of the short-lived conformers of ortho-substituted phenols using a population transfer IR-gain (PTIRG) spectroscopy for the first time. The details of PTIRG spectroscopy and how we found this exciting data for the ortho-substituted phenol systems will be presented.

Poster Presentation : **PHYS.P-295**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhanced Catalytic Dechlorination of 1,2-Dichlorobenzene Using Ni/Pd Bimetallic Nanoparticles Prepared by a Pulsed Laser Ablation in Liquid

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Bimetallic nanoparticles (NPs) exhibit advantageous electrical, optical, and catalytic properties. Among the various NP synthesis methods, pulsed laser ablation in liquid (PLAL) is currently attracting much attention because of its simplicity and versatility. In this study, a pulsed laser was used to produce nickel/palladium (Ni/Pd) bimetallic NPs in methanol and deionized water. The morphological and optical properties of the resulting Ni/Pd bimetallic NPs were characterized. The synthesized Ni/Pd bimetallic NPs were used for the dechlorination of 1,2-dichlorobenzene (1,2-DCB) under various conditions. The dechlorination rates of 1,2-DCB while using single (Ni and Pd) and bimetallic (Ni powder/Pd and Ni/Pd) NPs were investigated. The results showed that the Ni/Pd bimetallic NPs with 19.16 wt.% Pd exhibited much enhanced degradation efficiency for 1,2-DCB (100% degradation after 30 min). Accordingly, the results of enhanced the degradation of 1,2-DCB provide plausible mechanism insights into the catalytic reaction.

Poster Presentation : **PHYS.P-296**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of RuO₂ nanorods on electrospun WO₃ nanofibers

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Ruthenium oxide (RuO₂) nanorods on Tungsten oxide (WO₃) nanofibers were synthesized by combining the electrospinning method and a simple precipitation and recrystallization process. Crystalline structures and surface properties of synthesized nanofibers were characterized by scanning electron microscopy (SEM), Raman spectroscopy and X-Ray diffraction (XRD). In the synthesized RuO₂ - WO₃ nanofibers, it is shown that single crystalline RuO₂ nanorods were grown on the electrospun WO₃ nanofibers. It is expected that the nanostructures of synthesized nanofibers are critically affected by the annealing temperature and mass ratio of precursors. Ruthenium is a noble metal and has good electrochemical properties. It is reported that synthesized Ru@C₂N catalyst is an efficient, stable electrocatalyst for the HER in both acidic and alkaline media and comparable to Pt catalyst. Tungsten oxide is a widely used catalysts for its earth-abundance and cheap price. The synergistical interaction between ruthenium and tungsten powder has been reported to enhance the HER catalytic properties of ruthenium-tungsten composite catalyst made by simple physical mixing. Thus, the composite nanostructures between RuO₂ and WO₃ are expected to increase electrocatalytic and electrochemical activity than their single-phase nanostructures.

Poster Presentation : **PHYS.P-297**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Temperature dependence of dissociation constants for phenol red and piperazine-N,N'-bis(2-ethanesulfonic acid) using spectrophotometric method.

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Many aqueous systems with acid-base equilibria have been studied by a variety of analytical methods including potentiometric, conductimetric titration, fluorescence spectroscopy and chromatography. One of those, spectrophotometric methods using optical indicator have advantages of taking a minimum time, low cost and reducing the problems associated with different methods. In this work, we used spectrophotometric method to show the temperature dependence of dissociation constant for piperazine-N,N'-bis(2-ethanesulfonic acid) (PIPES). First, phenol red was used as the optical indicator to determine the acid-dissociation constant (K_a) in the phosphate buffer system. It exhibits two forms of protonated form, HIn^- (acidic absorption maximum at 443nm) and deprotonated form, In^{2-} (basic absorption maximum at 558nm) in aqueous solution. Dissociation constants of phenol red were calculated by ideal concentration ratio of acid-base obtained from deconvolution of absorption spectra and concentrations of phosphate buffer solutions. It was measured by temperature from 10 °C to 55 °C. Second, the dissociation constants of PIPES buffer system were calculated using determined dissociation constants of phenol red in first experiment. The experimental values of $\text{p}K_a$ were fitted to temperature dependent equation. Additionally, the dissociation constants of buffer solutions can be compared with values obtained by other methods. It will be conducted repeatedly for accuracy and precision of experiment.

Poster Presentation : **PHYS.P-298**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The New One-Dimensional Material Nb₂Se₉: Theoretical prediction of indirect to direct band gap transition due to dimensional reduction

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Many transition metal dichalcogenides (TMDCs) can have two-dimensional (2D) nanosheets structures, and decreasing the thickness of the sheets often changes their indirect band gap into direct band gap. Recently, a new one-dimensional (1D) semiconducting material Nb₂Se₉ was synthesized by solid-state reaction. This material consists of single-chain atomic crystals (SCACs) stacked periodically. To investigate the future application of this 1D material, we found the material properties by theoretical calculation. Firstly, we performed geometric optimization to Nb₂Se₉ bundles having 1-7 single units using density functional theory. We obtained band structures of all bundle systems and they had a direct band gap whereas the bulk Nb₂Se₉ had an indirect band gap. We predicted that the direct band gap occurred up to 21 SCACs bundles by interpolation of band gap change by the number of chains. Therefore, we expect that a Nb₂Se₉ SCACs whose diameter is less than 3.6 nm can cause electronic transition without the interaction between vibrational motions and be applied to photoluminescence.

Poster Presentation : **PHYS.P-299**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Computational study on the stability of oxygen vacancy in the ultrathin rutile TiO₂ film supported by a metal substrate

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Titanium dioxide (TiO₂) has a wide variety of applications such as photocatalysis and solar energy conversion. In particular, the oxygen vacancy receives a great attention because it plays crucial role in determining its chemical and physical properties. In this study, we perform dispersion-corrected density functional theory using projected augmented wave (PAW) method to investigate the stability of an oxygen vacancy in the ultrathin rutile titanium dioxide film supported by a metal substrate, TiO₂(110)/M(100) (M = body-centered cubic transition metal). The model system was constructed as *n*-ML rutile TiO₂(110) film (*n* = 1-3) supported by (2x1)-M(100) substrate, in which the lattice mismatches between TiO₂ and metal substrate for long and short axes are 1.52~13.44% and 2.31~10.30%, respectively. The stability of oxygen vacancy depending on its position was examined in order to provide insights into the formation of oxygen vacancy in a controlled manner.

Poster Presentation : **PHYS.P-300**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Theoretical prediction of oxidation mechanism of sulfurous acid by hydrogen peroxide

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At present time, people are facing large varieties of environmental problems. One of them is the presence of sulfuric acid (H_2SO_4). In the atmosphere, one of the possible pathways of H_2SO_4 formation is via the oxidation of H_2SO_3 . The latter is assumed to originate from abundant SO_2 and moisture. Recently, a mechanism of H_2SO_3 formation on the ice surface in application to low temperatures has been described. Also, the rise of H_2O_2 concentration in polar core ice during last decades has been observed. To the best of our knowledge, the detailed molecular mechanism of H_2SO_4 formation from H_2SO_3 has been poorly investigated. Thereby, we suggest possibility of oxidation of H_2SO_3 by H_2O_2 on the ice surface. Here, ab initio gas phase calculations have been done with aim to understand the mechanism of H_2SO_4 formation by oxidation of H_2SO_3 with H_2O_2 . Three different reaction pathways have been found. The first pathway proceeds via dissociation of H_2O_2 , the second occurs via peroxy intermediate $\text{HOSO}(\text{OOH})$, and the third takes place via another peroxy intermediate $(\text{HO})_3\text{S}(\text{OOH})$. The latter has not been reported previously in the literature. Additionally, it has been demonstrated that the presence of a water molecule will decrease the reaction barrier by as much as 16.0 kcal/mol. Further, ice surface calculations have been carried out and the results are discussed.

Poster Presentation : **PHYS.P-301**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

2D IR spectroscopy reveals picosecond interconversion between $n \rightarrow \pi^*$ interactions and hydrogen bonding in aqueous solution

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The delicate balance between multiple non-covalent interactions orchestrates the structure-function relationships in chemical and biological systems. $n \rightarrow \pi^*$ interactions involving electron delocalization from an oxygen lone pair (n) to the antibonding π^* orbital of either another carbonyl ($n \rightarrow \pi^*_{C=O}$) or an aromatic ring ($n \rightarrow \pi^*_{ar}$) have been implied to play prominent roles in the stability of bio-macromolecules, neurotransmitters, small drug molecules, and materials. To date, the $n \rightarrow \pi^*$ interactions have been characterized from theoretical calculations and crystal structure analyses, but little has been known regarding their coexistence and dynamic interplay with hydrogen-bonding interactions in solution. Here, using ultrafast two-dimensional infrared spectroscopy, we show that the strong hydrogen-bond and the weak $n \rightarrow \pi^*$ interaction coexist and interconvert in aqueous solution. We found that the kinetics of these interconverting interactions becomes faster with increasing water content. This experimental observation provides a new perspective on the existence of weak non-covalent interactions in aqueous solution.

Poster Presentation : **PHYS.P-302**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Extrapolation Scheme to Calculate Quantum Chemical Potential Energy of OH Stretching in Water

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A procedure to calculate the complete basis set limits of electronic energy of water molecules is developed based on two levels of fitting scheme. A three-point fitting scheme with the energies computed at the levels of basis function, aug-cc-pVXZ for $X = 4-6$, is employed to obtain accurate energies of nine dimers of water molecules. To represent the convergence pattern of the three levels of energy, we consider three extrapolation functions, power, stretched exponential, and exponential functions. The three functions are found to work excellently to give accurate Hartree-Fock (HF) energies of water molecules. However, the three functions give slightly different values up to 1-2 mHartree for the complete basis limit of electronic correlation energy. Although the correlation energy plays a critical role in determining the potential energy curve of OH stretching, the energetic difference with respect to the choice of extrapolation function are found to be practically not reflected in the potential curve. Aiming for applying to a mixed quantum/classical theory, we found a strong correlation between the extrapolated energy and the energies calculated at the level of double and triple zeta basis functions. This enables us to reproduce the extrapolated energy from the latter energies with much cheaper computation.

Poster Presentation : **PHYS.P-303**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dynamic and reactive molecular dynamics simulations on metal-silicon interface by neural network potential

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As the semiconductor devices continued to scale-down to 10 nm size, the prediction power of conventional device process simulation tools began to fail, due to their limitations with describing atomistic and quantum mechanical effects which become dominant in nano-meter-scales processes. For the reason, a new device/process simulation tool that can cover the atomistic pictures of the device processes is needed. While the density functional theory (DFT) calculation provides highly accurate information about material properties, its application is still limited to a few pico-seconds molecular dynamics (MD) simulations with several hundred atoms. With classical force fields, one can handle much larger systems up to million atoms and several nanoseconds. Thus, the simulations for semiconductor device process may be possible. However, the accuracy of classical MD simulations critically depends on the interatomic potentials. Although several classical potentials are poised to be highly accurate and transferable, optimizing the parameters in the force field requires strenuous efforts. Recently, neural network based potential (NNP) are gaining much attention. A NNP is constructed through the machine learning on the reference ab initio data. Since NNs can provide efficient and promising models for the arbitrary functional forms between given atomic coordinates and its potential energy surface, it gives interatomic potential that shows accuracy comparable to DFT. In this presentation, we tested and developed a NNP for simulating the formation of self-aligned nickel silicide. We collected the NNP training set which included various Ni-Si phases and Ni/Si interfaces. The result suggests that NNP simulation can be a powerful tool for atomistic device simulation.

Poster Presentation : **PHYS.P-304**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Revealing the effect of point defects on the shear exfoliation of nanoplates with thermodynamic free energy and Bernal-stacked conformation intermediate stability

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Since crystallographic defects are unavoidable in all crystalline materials in nature, we focus on the shear exfoliation of nanoplates with a few defects to deal with such problems. We perform extensive molecular dynamics simulations to consider the thesis in terms of macromolecular thermodynamic free energy and reaction kinetics. At first, we introduce point defects in nanoplates and calculate free energy to show the energetic change and stability of Bernal-stacking intermediates. Obviously, with defects, the energy cost required to exfoliate bilayer nanoplates decreases because of the reduction of the number of Van der Waals interaction pairs due to missing particles. On the other hand, the stability of intermediate states for different Bernal-stacked conformation reduces a lot and this change eliminates the free energy wells at the intermediate states. Based on our previous research, stable intermediate states facilitate the shear exfoliation. However, due to the destabilization of intermediate states, production rate of exfoliation drops. We next confirm that the nanoplates with a single defect are also more resistant to the shear. Under the same free energy cost, nanoplates with defects need 1.6 times stronger shear is required to exfoliate them completely. Consequently, we observe that the stability of intermediate states is crucial to the shear exfoliation of nanoplates.

Poster Presentation : **PHYS.P-305**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Effect of Nanogap Morphology on Plasmon Coupling in Nanocube-Nanosphere Dimers

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Plasmon coupling between two nanoparticles in close proximity tunes the optical resonance, depending on the extent of the interaction. Plasmon coupling is also responsible for the generation of strong electric fields in nanogaps, which is the fundamental basis of surface-enhanced Raman scattering (SERS). Therefore, understanding the plasmon coupling between two strongly interacting nanoparticles is not only academically appealing, but also practically useful for the rational design of plasmonic materials suited to color pixels, SERS substrates, and metal materials. Many experimental studies have focused on changing the gap distance as an adjusting parameter for the plasmon coupling. The effect of nanogap morphology has been overlooked. In this study, we explore how the morphology of nanogaps modifies the plasmon coupling between two nanoparticles. We prepare gold nanospheres (AuNSs) and nanocubes (AuNCs) and successfully assemble those particles into hetero dimers (AuNC–AuNS) using the masked desilanization method [1]. AuNC–AuNS dimers form various geometric isomers; AuNSs are attached to the face, the edge, or the corner of AuNCs. We measure plasmon coupling in those dimers that have different nanogap morphologies at the single-particle level. And we measure plasmon coupling using polarizer. In hetero dimer(AuNC-AuNS), depending on the polarization, the degree of feeling of the wavelength is different. We doing comparison of the experimental results with the finite-difference time-domain (FDTD) simulation. But experimental results and simulation results is not same. Because the two results are not exactly same environment (morphology/location of AuNS on AuNC/ shape/size). So we do modeling about AuNC-AuNS dimers and FDTD simulation close the experimental system. We reveal the nature of the plasmon coupling for various shapes (curvatures) of nanogaps. **ACKNOWLEDGMENTS** We gratefully acknowledge the support of this work by the National Research Foundation (NRF) of Korea (Grant No. 2016R1A2B2007259). **REFERENCES** [1] Cha H, YoonJH, Yoon S ACS Nano2014;8:8554.

Poster Presentation : **PHYS.P-306**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

DFT Study of Binding Affinity of a Bis-pyridinium Calix[4]pyrrole Derivative to Pyrophosphate and Chromenolate Anions

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A new bis-pyridinium calix[4]pyrrole derivative forms a non-fluorescent complex upon exposure to the chromenolate anion. The resulting supramolecular ensemble binds the pyrophosphate anion with high affinity in acetonitrile, leading to the recovery of fluorescence by the chromenolate anion separated from the supramolecular ensemble. It represents sensitive “turn-on” fluorescence when exposed to tetrabutylammonium pyrophosphate. In order to understand the supramolecular structure and binding affinity at the molecular level, we performed the DFT calculations. Electronic energies, structures, NMR chemical shifts, and thermodynamic properties for the bis-pyridinium calix[4]pyrrole derivative with pyrophosphate and chromenolate anions were acquired from this study and they were compared with experimental results. Our calculations identified a more stable structure among the possible supramolecular structures of calix[4]pyrrole derivative with pyrophosphate anion. In addition, the binding free energy calculations support the proposed “turn-on” fluorescence mechanism of the supramolecular system.

Poster Presentation : **PHYS.P-307**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Thermodynamic Behaviors of an Antimicrobial Peptide into Cell Membranes: A Molecular Dynamics Simulation Approach

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Due to its potential antibiotic properties, antimicrobial peptides (AMPs) have drawn much attention. In this study, we used all-atom (AA) and coarse-grained (CG) molecular dynamics (MD) simulations to investigate the interaction of small AMPs with gram-negative bacterial cell membranes composed of POPE and POPG lipid molecules. To investigate the effect of proline residue on the insertion of AMPs into the bacterial cell membrane, the potential of mean force (PMF) calculations for the AMPs with or without proline residue are performed using the umbrella sampling (US) and thermodynamic integration (TI) methods. The PMF profiles from the AAMD demonstrate that the AMP with the proline residue has better penetration efficiency into the bacterial cell membranes than the one without the proline moiety. The PMF curves from the both AAMD and CGMD simulations also show that the free energy minima of the AMPs are located near the lipophilic hydrocarbon region just below the hydrophilic headgroup region.

Poster Presentation : **PHYS.P-308**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Vibrational Circular Dichroism Spectroscopy of Jet-cooled Chiral Molecules

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Vibrational circular dichroism (VCD) refers to the differential absorption for left-handed and right-handed circularly polarized light (LCP and RCP, respectively) in the infrared (IR) region. VCD spectroscopy has been used to probe the chirality of molecular vibrations and the structures of chiral molecules. However, most of the VCD spectra have been measured in condensed phase, where the interactions between molecules, especially those with solvent molecules, make it hard to draw the structural information from the spectra. Here, we have developed a VCD spectroscopic technique applicable to gas-phase chiral molecules produced in a supersonic jet. The jet-cooled chiral molecules were irradiated with a circularly polarized IR laser pulse and then a linearly polarized UV laser pulse for resonance-enhanced multiphoton ionization. VCD spectra were obtained by monitoring the difference between the ion signals produced with IR-LCP and IR-RCP laser pulses as a function of the IR wavelength. Using this technique, we measured the VCD spectra of (-)- and (+)-Ephedrine near the OH stretching vibrational band.

Poster Presentation : **PHYS.P-309**

Physical Chemistry

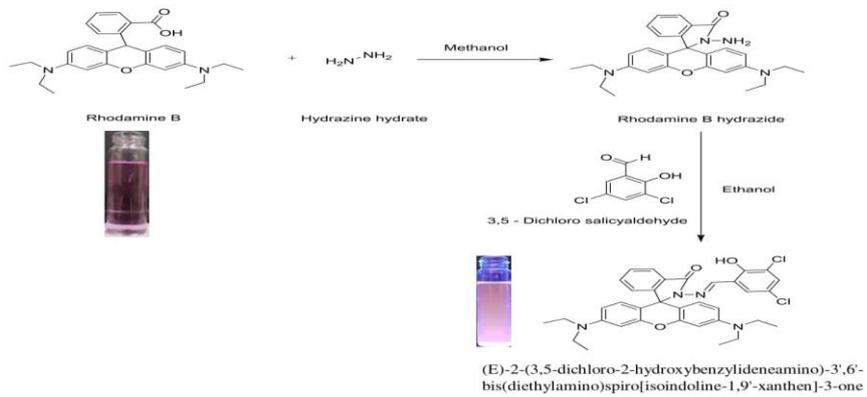
Grand Ballroom, FRI 11:00~12:30

Synthesis and photophysical properties of a rhodamine based fluorescence compound for its analytical application

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The present study deals with the design, synthesis, structural characterization, and photophysical properties viz. absorption and fluorescence of rhodamine derivative. The target compound was synthesized by condensing rhodamine B, hydrazine hydrate and 3,5-dichloro salicylaldehyde in alcohol as solvent. The structural characterization of compound was done by using ¹H NMR, IR and Mass spectroscopies. The synthesized compound showed excellent absorption and fluorescence properties as compared to the parent compound i.e. rhodamine B. The newly synthesized rhodamine derivative represent a new type of fluorescent material with efficient visible absorption and surpassing brightness which could be a promising candidate for chemo sensing, bioimaging, photonic applications, organic light emitting diodes and dye sensitized solar cells. References: 1. Dhara A, Jana A, Guchhait N, Ghosh P, Kat SK, New J. Chem. 2014; 38:1627-1634. 2. Saleem M, Abdullah R, Ali A, Park BJ, Choi EH, Hong IS, Lee KH, Bioorg. Med. Chem. 2014; 22:2045-2051.



Poster Presentation : **PHYS.P-310**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

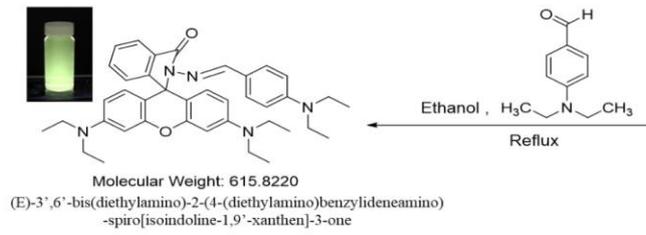
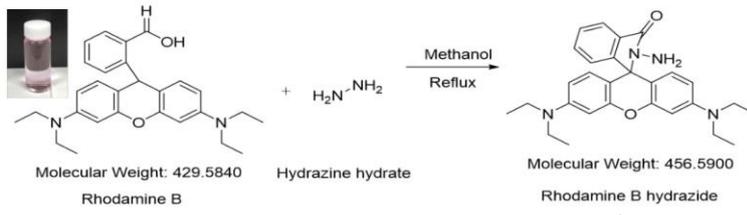
Synthesis of a simple Schiff base derivative based on rhodamine, its photophysical property and utility as chemosensor

Chae Won Lee, Prasad Gajanan Mahajan¹, Balasaheb Daniyal Vanjare¹, Ki Hwan Lee^{1,*}

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¹Department of Chemistry, Kongju National University, Korea

A simple Schiff base compound of rhodamine B was synthesized followed by their structural characterization, and photophysical properties viz. absorption, fluorescence and fluorescence lifetime studies. The schiff base derivative of rhodamine B namely (E)-3',6'-bis(diethylamino)-2-(4-(diethylamino)benzylideneamino)spiro[isoindoline-1,9'-xanthen]-3-one was derived from reaction between rhodamine B, hydrazine hydrate and p-diethylamino benzaldehyde in alcohol as solvent. The structural characterization of compound was done by using ¹H NMR, IR and Mass spectroscopies. The synthesized compound showed excellent absorption, fluorescence and fluorescence lifetime properties as compared to the parent compound i.e. rhodamine B. The newly synthesized Schiff base derivative based on rhodamine can be useful to direct application in various scientific areas such as bioimaging, chemosensors and electronic devices. References: 1. Mahajan PG, Dige NC, Desai NK, Patil SR, Kondalkar VV, Hong SK, Lee KH, Spectrochim. Acta A, 2018; 198:136-144. 2. Saleem M, Abdullah R, Ali A, Park BJ, Choi EH, Hong IS, Lee KH, Bioorg. Med. Chem. 2014; 22:2045-2051.



Poster Presentation : **PHYS.P-311**

Physical Chemistry

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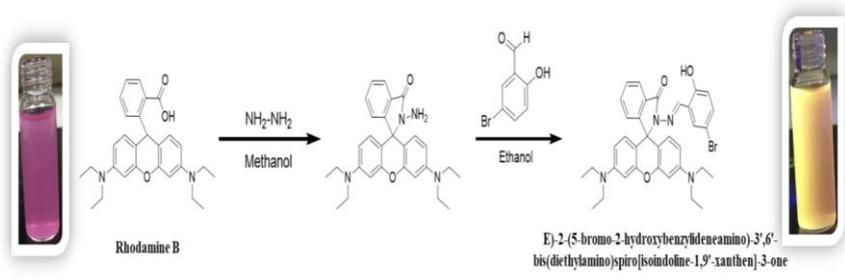
Synthesis of a simple schiff base derivative based on rhodamine and its utility as analytical probe

**Han Sol Hong, Jeong Pyo Hong, Prasad Gajanan Mahajan¹, Balasaheb Daniyal Vanjare¹,
Ki Hwan Lee^{1,*}**

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The new fluorescent rhodamine derivative namely (E)-2-(5-bromo-2-hydroxybenzylideneamino)-3',6'-bis(diethylamino)spiro[isoinoline-1,9'-xanthen]-3-one has been synthesized. The studies on its photophysical properties are the other main part of our present study. The desired rhodamine derivative was synthesized via condensation reaction of rhodamine B, hydrazine hydrate and 5-bromo salicylaldehyde in alcohol as solvent at reflux conditions. The spectral characterization of synthesized compound was done by using ¹H NMR, IR and Mass spectroscopies. The excellent photophysical properties possessed by synthesized derivatives signifies it can be useful as far as application in chemo sensing and biomarker in environmental and biological studies. References: 1. Vanjare BD, Mahajan PG, Hong SK, Lee KH, Bull. Kor. Chem. Soc. 2018; 39:631-637. 2. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer US, New York, 2006. 3. Saleem M, Abdullah R, Ali A, Park BJ, Choi EH, Hong IS, Lee KH, Bioorg. Med. Chem. 2014; 22:2045-2051.



Poster Presentation : **PHYS.P-312**

Physical Chemistry

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Synthesis and characterization of rhodamine based Schiff base derivative owning to photophysical properties and application

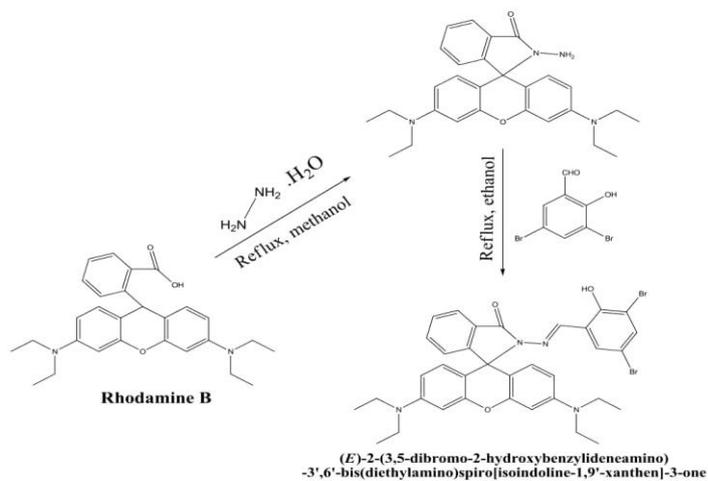
**Kyou Yeong Sim, Jungsuk Shin¹, Prasad Gajanan Mahajan², Balasaheb Daniyal Vanjare²,
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The condensation approach has been used to derive a rhodamine based Schiff base derivative namely (E)-2-(3,5-dibromo-2-hydroxybenzylideneamino)-3',6'-bis(diethylamino)spiro[isoindoline - 1,9'-xanthen]-3-one. For this purpose reaction between rhodamine B, hydrazine hydrate and 3,5-di-bromosalicylaldehyde has been carried out in alcohol at reflux condition. The spectral purity and confirmation of synthesized compound was done by using ¹H NMR, IR and Mass spectroscopies. The studies on absorption, fluorescence and lifetime decay signifies that synthesized derivative has superior photophysical properties than parent molecule i.e. rhodamine B. The possible application fields for synthesized rhodamine based Schiff base derivative are heavy metal ion sensing, cell imaging, biomarker, etc. due to its photophysical properties. References: 1. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer US, New York, 2006. 2. Saleem M, Abdullah R, Ali A, Park BJ, Choi EH, Hong IS, Lee KH, Bioorg. Med. Chem. 2014; 22:2045-2051.



Poster Presentation : **PHYS.P-313**

Physical Chemistry

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A new fluorescein based organic nano probe for Selective and Sensitive detection of Cu²⁺ in aqueous media

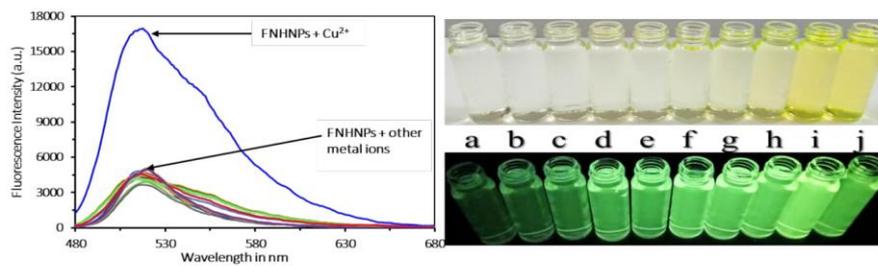
Prasad Gajanan Mahajan, Nilam C. Dige¹, Balasaheb Daniyal Vanjare, Seong-Karp Hong², Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

¹*Chemistry, Shivaji University, India*

²*Department of Biomedical Engineering, Mokwon University, Korea*

A fluorescein based organic nanoparticles were prepared by using N-(3',6'-dihydroxy-3-oxo-3,3a-dihydrospiro[isoinidole-1,9'-xanthene]-2(7aH)-yl)-1-naphthamide (FNH). The interaction of series of metal ions with the FN nanoparticles (FNHNPs) was investigated by means of fluorescence measurement. The selective and sensitive fluorescence enhancement was observed to FNHNPs by the addition of Cu²⁺ ion in an aqueous medium. The interaction of FNHNPs and Cu²⁺ introduced chelation enhanced fluorescence that was unaltered even addition of other metal ion. The formation of excited state complexation of FNHNPs-Cu²⁺ was supported by UV-vis absorption titration, fluorescence lifetime and zeta particle size of FNHNPs with and without addition of Cu²⁺. The stoichiometry and binding constant estimated by Job's plot and modified Benesi-Hildebrand plot. The limit of detection (LOD) for Cu²⁺ was 1.62 ng/mL. The fascinating feature of present nano probe (FNHNPs) is that outstanding intracellular Cu²⁺ sensor in living cells. The exceptional photophysical and biocompatible nature of FNHNPs signifying on site application of prepared fluorescent organic nanoparticles in environmental as well as biomedical field. References: 1. Xiang Y, Tong A, Jin P, Ju Y, Org. Lett. 2006; 8:2863-2866.2. Saleem M, Lee KH, J. Lumin. 2014; 145:843-848.3. Royzen M, Dai Z, Canary JW, J. Am. Chem. Soc. 2005; 127:1612-1613.



a-FNH in acetone, **b**-FNHNPs, **c**-FNHNPs + 2 $\mu\text{g/mL}$ Cu^{2+} , **d**-FNHNPs + 4 $\mu\text{g/mL}$ Cu^{2+} , **e**-FNHNPs + 8 $\mu\text{g/mL}$ Cu^{2+} , **f**-FNHNPs + 12 $\mu\text{g/mL}$ Cu^{2+} , **g**-FNHNPs + 16 $\mu\text{g/mL}$ Cu^{2+} , **h**-FNHNPs + 20 $\mu\text{g/mL}$ Cu^{2+} , **i**-FNHNPs + 24 $\mu\text{g/mL}$ Cu^{2+} , **j**-FNHNPs + 28 $\mu\text{g/mL}$ Cu^{2+} .

Poster Presentation : **PHYS.P-314**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis, Photophysical properties and Bio-imaging application of Novel Rhodamine based derivatives

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¹Department of Biomedical Engineering, Mokwon University, Korea

Rhodamine dyes usually used as fluorescent probe owing to their high absorption coefficient, broad fluorescence in the visible region of electromagnetic spectrum, high fluorescence quantum yield and photostability. Herein, we synthesized a novel fluorescent derivatives based on Rhodamine B. In order to compare the fluorescence properties of these dyes, the spectroscopic properties in different solvents were comprehensively studied. The formation and purity of the synthesized probes RHB1, RHB2 and RHB3 were confirmed by using analytical techniques viz. ¹H NMR, ¹³C NMR, Mass and FT-IR followed by investigation of spectroscopic properties such as UV-vis absorption spectroscopy, fluorescence spectroscopy and fluorescence quantum yield. In addition, the cancer cell (MBA-MD-231) treated with the synthesized probes RHB1, RHB2, and RHB3. It is clear from the result of the conventional fluorescence microscopy and cytotoxicity that, RHB2 dye having more fluorescence compared with RHB1 and RHB3. References: 1. Chen. J, Liu W, Zhou B, Niu G, Zhang H, Wu J, Wang Y, Ju W, Wang P, J. Org. Chem. 2013; 78:121–130. 2. Bozkurt E, Gul H, Mete E, E, Journal of Photochemistry and Photobiology A: Chemistry, 2018; 352:35–42. 3. Yang K, Leslie K, Kim S, Kalionis B, Chrzanowski W, Jolliffe K and New E, Org. Biomol. Chem., 2018; 16:619- 624.

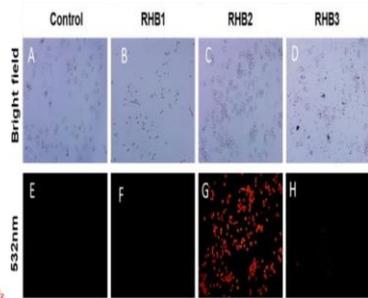
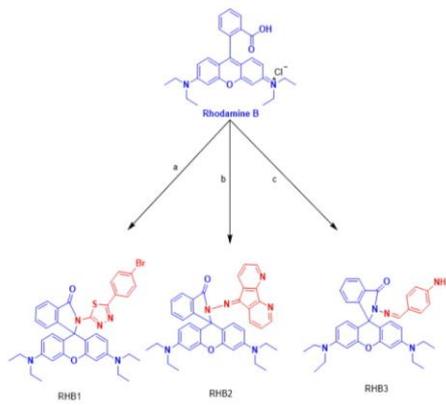


Fig 4: Bright field transmission images of MDA-MB-231 cells with control (A), RHB1 (B), RHB2 (C), and RHB3 (D) and fluorescence images of living MDA-MB-231 cells with control (E), RHB1 (F), RHB2 (G), and RHB3 (H) at 532 nm.

Poster Presentation : **PHYS.P-315**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

NiFe layered double hydroxide nano-sheets on CdS solar driven Photocatalytic hydrogen production rate synthesized through Liquid phase Pulsed laser ablation

**Hwan Lee, Amaranatha Reddy¹, Yujin Kim¹, Rory Ma¹, Praveen Kumar Dharani¹,
TaeKyu Kim^{1,*}**

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Molecular hydrogen evolution based on solar driven semiconductor is one of the best ways for creating green fuel. However, this process has limit such as high cost semiconductor nanostructures, low stability and efficiency. The noble-metal-free CdS-NiFe LDH nanocomposite is a efficient solar driven photocatalyst, which has the unique 2D NiFe LDH nanosheets-on- 1D-CdS nanorod heterostructure. This heterostructured close interfacial contact not only allows for more efficient photocharge carrier transport and migration due to their suitable reduction potentials than that of bare CdS, but also greatly reduces the recombination rate. Futhermore, it also provides a large number of catalytically active sites for hydrogen production reaction due to its ultra-thin flexible nature and effectively broad surface area. As a result, the fabricated CdS/NiFe nanocomposite exhibits a high hydrogen evolution rate of 72 mmol g⁻¹ h⁻¹, which surpasses that of most nanocomposites previously reported in literatures on various CdS-based co-catalyst nanostructures. We expect that the demonstrated methodology for the fabrication of noble metal free CdS-based co-catalyst nanostructures and their application in photocatalytic hydrogen evolution may lend novel insights to promote cost-effective photocatalysts for H₂ production.

Poster Presentation : **PHYS.P-316**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Infrared spectroscopy of Aniline and Phenol gases: background free ion-gain IR after IVR process and ion-loss IR after a burning of populations of the ground state

Heesung Lee, Sang Kyu Kim*

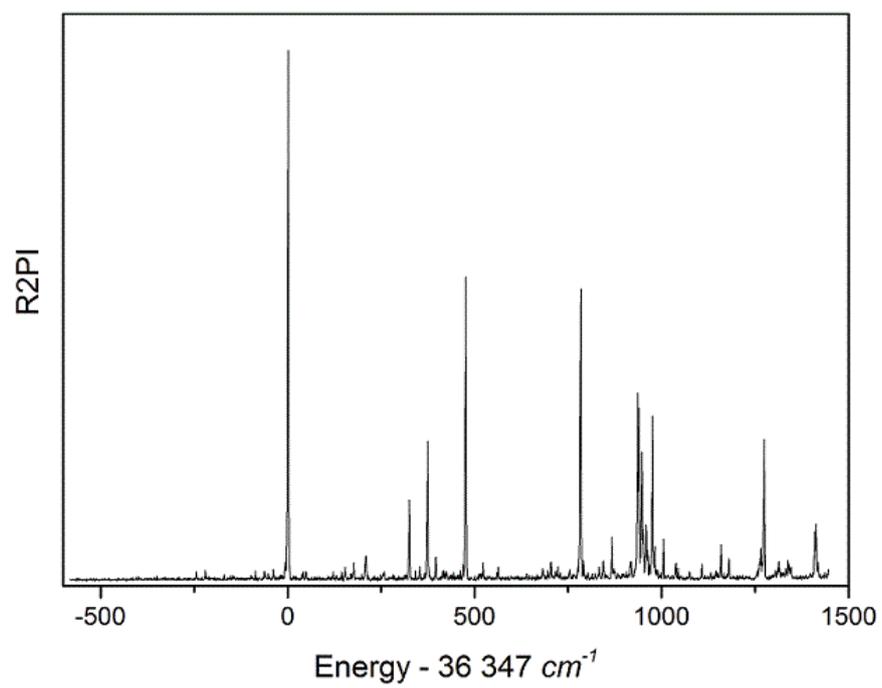
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

IR-UV double resonance spectroscopy for chemical dynamics had been widely studied for several decades. Nevertheless, the reported studies for the control of photo-fragmentations among the aromatic systems are rare because of an obstacle of intramolecular vibrational energy redistribution (IVR) within ps time scale. Instead, there are tremendous IR-UV studies for the goals of structural determinations of ground states of a number of chromophores. Here, our group tried to obtain IR-UV double resonance spectra for further dynamics study. There were benchmark works for the IR-UV spectroscopy before doing further dynamics studies [1,2,3]. In both cases, bath states due to the excitation of infrared laser beam allows the molecules to be excited to the ground ion state via induced S_1 resonance states. We obtained ion-gain IR (i.e. enhanced parent ion signals through IVR after IR introduction) as well as ion-dip IR (i.e. decreased parent ion signals due to the depletion of ground state populations) for those two molecules (Aniline and Phenol), respectively. Our results can be base for the future stereodynamics study.

[1] Chemical Physics Letters, 252, 287 (1996)

[2] International Journal of Mass Spectrometry 220, 289-312 (2002)

[3] The Journal of Chemical Physics 123, 124316 (2005)



Poster Presentation : **PHYS.P-317**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dual-wavelength lasing of InGaN/GaN heterostructure nanorods

So Yeon Chun

Department of Chemistry, Kyung Hee University, Korea

So Yeon Chun, Jae Kyu Song Department of Chemistry, Kyung Hee University, Seoul 130-701, Korea
Abstract One-dimensional (1D) semiconductor nanostructures can function as both the gain medium and optical cavity, which are suited for nanoscale lasers. The nanowire lasers have been reported for several homogeneous binary semiconductors, including GaN, ZnO, and CdS. In addition, the emission wavelength has been controlled by varying the elemental ratio of ternary semiconductors. However, the dual-wavelength laser from single nanowires has not been reported. We investigate dual-wavelength lasing of InGaN/GaN heterostructure nanorods. Interestingly, the lasing of InGaN around 520 nm shows the classical Fabry-Perot modes, whereas the non-classical mode spacing is observed in the lasing of GaN around 370 nm, suggesting the strong light-matter interactions.

Poster Presentation : **PHYS.P-318**

Physical Chemistry

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Effect of dye-labelling on the rotational dynamics fluorescence molecules in polymer

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Department of Chemistry, Sungkyunkwan University, Korea

The segmental dynamics of polymer is known to be closely related to the glass transition where the glass transition is the single most important parameter in its application. The segmental dynamics of polymers that leads to the glass transition can be studied by probing ensemble rotational motion of fluorescent molecules in polymers via a polarized fluorescence correlation approach. However, in previous research on the segmental dynamics of polymers near the glass transition, not only rotational motion of the fluorescent probes but also the translation motion can be present if fluorescent probes are not attached to the polymer. Therefore, we replace the terminal functional group of the fluorescent probes with an amine group and react fluorescent probes with a carboxylic acid terminated polymer to prevent translation motion of fluorescent probes while probing rotational motion of fluorescent probes. The rotational dynamics of polymer-labelled fluorescent probes was found to be slower than freely rotating fluorescent probes, but temperature dependence of rotational relaxation time of polymer-labelled fluorescent probes did not change upon labelling.

Poster Presentation : **PHYS.P-319**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Ratiometric pH-Sensor Based on Dye-conjugated Upconversion Nanoparticles

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Intra-cellular pH-sensing is of huge importance to understand the cellular activities and detection of diseases in an early stage. Therefore, the optical pH-nanoprobes that can work in biological environment, is an immediate requirement in medical research and diagnostics. In this work, the dye-conjugated upconversion nanoparticles (UCNP) have been prepared as pH-sensing system based on the based on fluorescence resonance energy transfer. We have analysed the variation of luminescence emission in ratiometric manner from the pH-dependent fluorescein dye and pH-insensitive NaYF₄: Tm³⁺/Yb³⁺ UCNPs to measure the pH of the system. The synthesized upconversion nanoparticles are useful for biological application, due to their low cytotoxicity, high photostability, low photobleaching and lack of autofluorescence in biological materials.

Poster Presentation : **PHYS.P-320**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Intermolecular Structural Differences of Poly(3-hexylthiophene) Probed by Polarized Raman Spectroscopy and Theoretical Calculation

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Department of Chemistry, Dong-A University, Korea

A conductive polymer, poly(3-hexyl-thiophene) has been widely used for photovoltaic applications. Its good conductivity is originated from polaron pair formation assisted by intramolecular pi-conjugated electrons in the backbone and intermolecular pi-pi interactions. These intra- and inter-molecular pi interactions may affect C=C and C-C Raman features shown at ~ 1370 and ~ 1450 cm^{-1} , since they are correlated to molecular structural orderings and randomness. Against these backdrops, here we have examined the depolarization ratio (r) of C=C and C-C vibration Raman modes of the ordered (annealed, $r \sim 0.3$) and disordered (non-annealed, $r \sim 0.2$) P3HT films. We also have confirmed that the depolarized ratio clearly reflects different intermolecular structures using MP2/6-31g(d, p) theory.

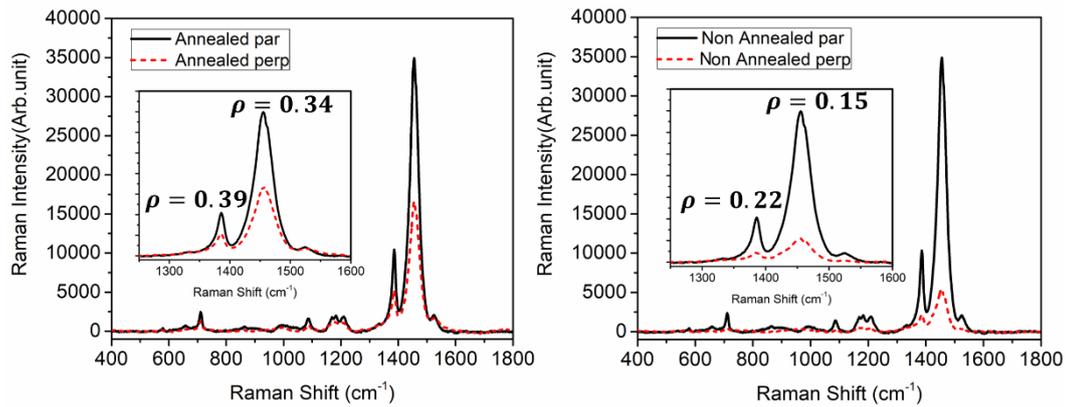


Figure 1. Raman spectra of annealed and non annealed P3HT.

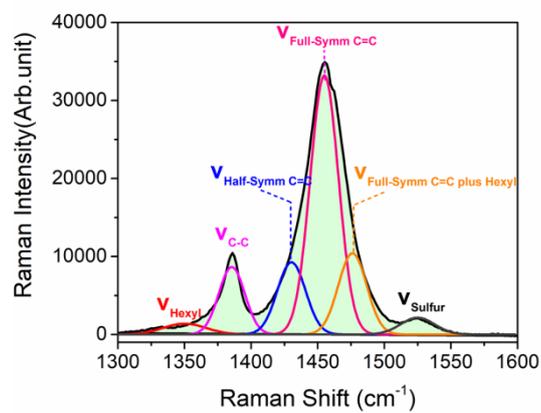


Figure 1. Raman peaks and assignment measured at 1460 cm^{-1} (C=C) and 1380 cm^{-1} (C-C)

Figure 2. Raman peak assignment measured at 1460 cm^{-1} (C=C) and 1380 cm^{-1} (C-C).

Poster Presentation : **PHYS.P-321**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Metal-Enhanced Fluorescence and Energy Transfer of Dyes Observed with Homogeneous Silver Colloidal Surfaces

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¹Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Korea

Metal-enhanced fluorescence (MEF) has been extensively applied to many research areas due to the strong enhancements in the fluorescence intensity and photostability. MEF has been described as arising from the local electric field enhancement and plasmon-coupled emission by the surface plasmon resonance (SPR) of metal nanoparticles. Recently, we observed the strong fluorescence enhancements based on the ultrafast energy transfer between dyes and silver island surfaces, but further studies were limited due to the inhomogeneity of the surfaces. In this work, homogeneous silver colloidal films (SCFs), composed of particles with a diameter from ~70 to 200 nm, were fabricated. The MEF and emission kinetics of DCM and Rh700 with SCFs were investigated by time-resolved fluorescence spectroscopy. The dipolar and multipolar SPR bands of SCFs were observed in a wide range of wavelengths depending on the particle diameter. The fluorescence of DCM and Rh700 was most strongly enhanced when the SPR bands of the SCFs overlap with the emission bands or exist between the absorption and emission bands of dyes. From the time-resolved fluorescence spectra and finite-difference time-domain simulations, the relative contributions of the electric field effect, plasmon-coupled emission, and fluorescence quenching were estimated. The fluorescence enhancements of these dyes originate predominantly from the electric field effect, but the particle size dependence in the enhancements arises mainly from the plasmon-coupled emission.

Poster Presentation : **PHYS.P-322**

Physical Chemistry

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Computational Study on the Structural and Thermodynamic Properties of SOD1

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*Nano/Bio Computational Chemistry Lab., Department of Chemistry, Sookmyung Women's University,
Korea*

Amyotrophic lateral sclerosis (ALS) is a selective dying disease of the spinal motor nerves. Although it is a progressive incurable disease, there is no proper treatment currently available. Excessive SOD1 and its mutants undergo protein aggregations in neurons, which are supposed to spread to adjacent cells, leading to the death of nerve cells. Therefore, the mutation of the SOD1 induces genetic ALS, and it is presumed that it plays a role in the sporadic type of non-genetic ALS disease. In this study, we investigate the effect of individual mutations on the structural and thermodynamic properties of the SOD1. We perform molecular dynamics simulations to probe structural changes induced by the mutations, and then carry out solvation free energy calculations to analyze thermodynamic features. Our study will contribute to an understanding of the SOD1 aggregation associated with ALS disease, and also provide the structural basis for developing drugs that inhibit the aggregation.

Poster Presentation : **PHYS.P-323**

Physical Chemistry

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The computational studies on the Binding Affinity properties of Stapled p53/HDM2 and Unstapled p53/HDM2 complexes

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Department of Chemistry, Sookmyung Women's University, Korea

The p53 tumor suppressor protein exerts antiproliferative effects, including growth arrest and apoptosis, in response to various types of stress pathways. In our body, p53 protein exists binding to HDM2 hence it will not active the tumor suppressor function. Therefore, the inhibition of p53/HDM2 interaction presents an appealing therapeutic strategy for the treatment of cancer. Previously, some developed structures have been constructed mimicking the epitope residues of p53 peptides and have been studied for their interaction with HDM2 proteins as well as hydrocarbon stapled peptides have found to make up a promising class of protein-protein interaction regulators. In this study, we report the structural and thermodynamic characteristics for the binding complex of the stapled p53/HDM2 and unstapled p53/HDM2. Moreover, we investigated the structural information of the complexes by molecular dynamics simulations. The binding free energy calculation based on the integral equation theory was also executed to quantify the binding affinity for the complex and to understand the factors of the binding affinity of the complexes. As a result, we found that the binding affinity of the stapled p53 peptide was higher than that for the corresponding unstapled peptide. We determined structurally and thermodynamically that the hydrocarbon linker contributes significantly to the high binding affinity of the stapled p53/HDM2.

Poster Presentation : **PHYS.P-324**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

The aqueous dynamics of CO₂ capturing by Quantum Mechanical Molecular Dynamics

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Department of Chemistry, Kyungpook National University, Korea

The aqueous dynamics of CO₂ capturing was investigated by quantum mechanical molecular mechanical molecular dynamics (QM/MM-MD) simulation. It is shown here that H₂CO₃ and NH₂COOH formations proceed with very high activation barriers in the gas phase. While in solution, not only the mechanism is different from the gas phase, but also the activation energy is decreasing in magnitude with catalysts.

Poster Presentation : **PHYS.P-325**

Physical Chemistry

Grand Ballroom, FRI 11:00~12:30

Plasmon-Driven Decarboxylation Reaction of 4-Mercaptobenzoic Acid in Nanogaps

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

Surface plasmon resonance (SPR) of noble metal nanoparticles has attracted considerable attention because of their wide range applications. Surface plasmons decay through either radiative or nonradiative pathways, where localized surface plasmon resonance (LSPR) can produce a huge electromagnetic field to get greatly enhanced Raman signal, the nonradiative relaxation pathway generates hot charge carriers and/or localized heating around nanoparticles which play a significant role in the plasmon-driven reactions. By using a easy fabricated nanoparticle-on-mirror (NPOM) system by adsorbing gold nanoparticles (AuNPs) on self-assembled monolayers (SAMs) on Au substrates, we study the mechanism of the plasmon-driven decarboxylation reaction of 4-mercaptobenzoic acid (MBA) in nanogaps. The reaction is monitored in situ by the SERS of molecules from these nanogaps which provides information with high sensitive. We discover that excitation of the coupled plasmon modes generates hot charge carriers in AuNPs. Interaction of hot charge carriers with carboxylate anion and proton at the surface of AuNPs leads to the formation of carboxylate and hydrogen radicals. This plasmon-driven process is unequivocally corroborated by dependence of reaction rate on the excitation wavelengths. Blocking the transport of hot charge carriers inhibits the reaction. The carboxy radical undergoes the homolytic cleavage process in the MBA, leading to the formation of BT and carbon dioxide products.

Poster Presentation : **PHYS.P-326**

Physical Chemistry

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Optically-active vibrational sum-frequency generation spectroscopy of chiral molecules in isotropic liquid

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¹*Korea Basic Science Institute, Korea*

Chiral molecule plays an important role in chemistry, biology and medicine, and its stereo-chemical structure sometimes critically affects its biochemical activity. Various chiroptical methods such as circular dichroism (CD), vibrational CD (VCD), and Raman optical activity (ROA) have been extensively used to determine stereo-specific structures of chiral molecules. Recently, we developed a chiral vibrational sum-frequency generation (VSFG) technique capable of distinguishing between optically-active vibrational features of enantiomers in isotropic liquid. By employing narrowband near IR and broadband mid-IR laser beams, we could obtain the chiral VSFG spectrum in the C-H stretching frequency region of limonene without any frequency scan of the mid-IR beam. It was found that the circular intensity difference (CID) SFG signal is highly sensitive to the vibrational optical activity of two different enantiomers with opposite chirality, allowing distinguishing between them. We also studied the polarization-dependence of the chiral, achiral and CID SFG spectra and found that different polarization combinations of the mid-IR, near-IR and SFG beams lead to the generation of the SFG signals associated with different hyperpolarizability tensors and their interference.

Poster Presentation : **ANAL.P-327**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Sol-Gel Matrix for the Development of a Thiocyanate-Selective Membrane Electrode

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Chemistry, Inje University, Korea

¹*Department of Chemistry, Inje University, Korea*

In an effort to prepare thiocyanate-selective chemical sensors, an organic-inorganic hybrid sol-gel matrix was used as membrane host for an appropriate sensing material. Tricaprylylmethylammonium thiocyanate (Aliquat336-SCN) was employed as the dissociated ion-exchanger type sensing ionophore. The sol-gel precursor was obtained by the reaction of 3-isocyanatopropyltriethoxysilane with 1,4-butanediol. Being mixed with Aliquat336-SCN and an acidic catalyst, the sol-state precursor slowly gelled to give an Aliquat336-SCN-containing membrane. Tributylphosphate (TBP) was used as a plasticizer. Electrochemical performances of the sol-gel membrane-based electrodes were compared to those of Aliquat336-SCN-based poly(vinyl chloride)(PVC) membrane electrodes. Membranes with an optimum ratio of Aliquat336-SCN: sol-gel precursor (1.0: 9.1 by weight) showed very stable baseline potentials. On the 7th working day, an average response slope toward thiocyanate was approximately 56.3 mVdecade⁻¹ in the concentration range 10^{-4.5} and 5x10⁻¹ M at 20°C. Moreover, selectivity toward thiocyanate over salicylate and other lipophilic anions was significantly improved, deviating from the Hofmeister selectivity pattern which is observed in most dissociated ion-exchanger-based potentiometric membrane sensors. The selectivity coefficients measured by the separate solution method in 0.05 M MES buffer, pH 5.5, were $\log k^{\text{pot}}_{\text{thiocyanate, chloride}} = -2.3$, $\log k^{\text{pot}}_{\text{thiocyanate, salicylate}} = -0.6$, and $\log k^{\text{pot}}_{\text{thiocyanate, perchlorate}} = -0.1$. **Keywords:** Anion-selective membrane electrode, Sol-gel method, Thiocyanate

Poster Presentation : **ANAL.P-328**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

LC/MS/MS based Construction of Isomer-Specific and Region-Specific Mouse Brain Ganglioside Library

Jaekyung Yun, Hyun Joo An*

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

Gangliosides are anionic glycosphingolipids containing one to several sialic acid residues. Although they play an important role in neuro-biological functions including synaptic plasticity and memory formation, there have been only few studies in ganglioside due to their structural complexity and the lack of effective analytical methods. In particular, isomeric investigation of gangliosides is necessarily required in order to understand the ganglioside biology with the consideration of its biosynthesis however, isomer separation based on reversed-phase (RP) chromatography is highly challengeable. In this study, for the purpose of construction of localized mouse brain ganglioside library, we examined ganglioside from anatomically dissected nine mouse brain regions by isomer-specific LC/MS and LC/MS/MS. Briefly, gangliosides were extracted by modified Folch method with chloroform and methanol, followed by purification and enrichment by C18-SPE. Then they were identified and quantified by UHPLC (C18 column) QTOF MS. Ganglioside isomers were completely separated depending on their glycan traits on a C18 column by addition of formic acid in the mobile phase. Furthermore, tandem MS analysis was performed to confirm the identification based on diagnostic fragment ions. Approximately, isomeric structures of 40 ganglioside compositions were elucidated including O-acetylated species. Through LC-MS/MS based isomeric investigation of gangliosides, region-specific mouse brain ganglioside biosynthetic pathway including 0-, a-, b- and c- series could be suggested. Interestingly, major ganglioside were distributed with distinguished qualitative and quantitative pattern for each nine brain regions. Constructed mouse brain ganglioside library is going to be used for monitoring alteration in KO mouse models including glycosylation transferase KO mice.

Poster Presentation : **ANAL.P-329**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Analysis of polyglycerophospholipids using isotope-labeled methylation

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Polyglycerophospholipids (PGPLs) are divided into phospholipids (PLs) containing two glycerols including phosphatidylglycerol (PG), bis(monoacylglycero)phosphate (BMP), hemi BMP, and bis(diacylglycero)phosphate (BDP), and PLs with three glycerols such as cardiolipin (CL), monolysocardiolipin (MLCL), and dilyocardiolipin (DLCL). PGPLs are synthesized from PG and closely related to each other. Since PGPLs have been reported to be associated with neurodegenerative diseases, accurate determination of these lipids is important. Isotope-labeled methylation (ILM) method using (trimethylsilyl)diazomethane (TMSD) can be utilized for relative quantitation of lipids without the addition of internal standard lipids. In addition, many lipids of trace amount could be detected by ILM method with low detection limit. In this study, analysis of PGPLs with ILM method was carried out using nUHPLC-ESI-MS/MS. The collision-induced dissociation (CID) experiments was conducted for the methylated standard PGPLs. The efficiency of methylation for these lipids was found to be > 97% and the degree of methylation was dependent on the number of phosphate groups (1: PG, BMP, Hemi BMP and BDP, 2: CL, MLCL and DLCL). PG and BMP, which are geometrical isomers, and three isomers of BMP can be resolved from each other. A good linear relationship between experimental mixing ratio and calculated peak area of H-/D- methylated lipids were observed. This method was applied to the investigation of PGPLs from a neuronal cell line (SH-SY5Y) which was treated with some drugs, commonly used for the Parkinson's disease model, were quantitatively analyzed.

Poster Presentation : **ANAL.P-330**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Alteration of plasma lipidome among five representative cancers by nUHPLC-ESI-MS/MS

Gwang Bin Lee, JongCheol Lee, Myeong Hee Moon*

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Cancer is one of the critical social problems as the incidence grows every year. Causes of cancer are known to be genetic factors, regimen, and environment conditions and so on. Because of the complexity of the cause, it is very important to understand the cause of cancer more clearly. Lipid is one of the substances that play key roles in the metabolism of human bodies and also known to be associated with various cellular processes such as survival, proliferation, and death. These cellular processes are associated with cancer genesis pathways, especially to transformation, progression, and metastasis, suggesting that lipids are mediators of carcinogenesis processes. In a recent research, lipidomic analysis as regard to cancer attracts more interests since each type of cancer has different carcinogenesis pathways and characteristics. In this study, plasma lipids from 5 different types of cancer patients (liver, gastric, lung, colorectal, and thyroid cancers) were investigated in order to figure out lipids that show significant differences among the groups and to find potential lipid biomarkers of each cancer. Lipids were extracted from blood plasma sample using the modified Folch method with MTBE/methanol, and analyzed by nUHPLC-ESI-MS/MS. Overall, 357 lipids from patient's plasma with liver, stomach, lung, colorectal, thyroid cancer, and controls, were identified and 242 lipids were quantified by nUHPLC-ESI-MS/MS with statistical evaluations for the selection of candidate biomarkers.

Poster Presentation : **ANAL.P-331**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS

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Lipids are the basic building blocks of cell membrane and are the sources of energy production and the crucial signaling molecules in controlling metabolism through activating or deactivating protein kinases, hormones or related metabolites. With lipid alteration in aging, however, these regulation processes gradually lose their control, and then eventually result in age-related diseases such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Although a number of studies have been conducted to reveal the relationship between age-related diseases and lipids, only few studies have compared lipid changes with aging effect. In this study, lipid profiles in serum, kidney, and heart from C57BL/6 aging mice were examined to understand aging effect solely. Genetically well-controlled and raised 4 and 25-month-old mice which represent young and aged were analyzed by nanoflow ultrahigh pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Above 350 lipid species were identified from each sample group and 163 from serum, 210 from kidney, and 202 from heart were quantified with internal standards of each class. From quantification, most significantly changed (> 1.5 fold and $p < 0.01$) lipid species were found to be down-regulated by aging, but PG and TG species were distinctively up-regulated in heart.

Poster Presentation : **ANAL.P-332**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Profiling of oxidized phospholipids in exosome and subcellular species of cells under oxidative stress by flow field-flow fractionation and nUHPLC-ESI-MS/MS

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Oxidative stress occurs when production of reactive oxygen species (ROS), which include oxygen derived radical species such as superoxide anion (O_2^-) and hydroxyl radical ($\cdot OH$) as well as hydrogen peroxide (H_2O_2), exceeds removal capacity of antioxidants. Moderate concentration of ROS is related to some beneficial physiological roles (e.g. signaling, host defense), but high levels of ROS not only induces cellular impairments by altering DNA, RNA, proteins, and lipids but also involves with a number of diseases like cardiovascular disease (CVD) or cancer. Exosomes are nano-sized extracellular vesicles secreted from cells. It has been reported that exosome transports some protective RNA against oxidative stress or transfers stress signals to recipient cells, when oxidative stress is given to cells. However, physiological roles or changes of lipids in exosome during oxidative stress conditions have not yet been studied. In this study, oxidative stress was induced to human embryonic kidney cell 293 (HEK293) by treating with H_2O_2 for 72 hours. Exosome and cellular organelles from control and oxidatively stressed conditions were size-sorted by flow field-flow fractionation first. Then, changes in lipid profiles in cell and exosome was conducted by nUHPLC-ESI-MS/MS.

Poster Presentation : **ANAL.P-333**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Separation of lipoproteins and exosome in plasma using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

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Department of Chemistry, Yonsei University, Korea

Lipoproteins transport hydrophobic molecules such as cholesterol in blood and are known to be associated with diseases such as arteriosclerosis. Lipoproteins are classified by high-density lipoprotein (HDL, 5~15 nm), low-density lipoprotein (LDL, 18~28 nm), very low-density lipoprotein (VLDL, 30~80 nm) according to its size and density. Exosomes are extracellular vesicles secreted by cells and their sizes are known as about 30~150 nm in diameter, which are larger than LDL but similar or slightly larger than VLDL. Exosomes are known to play an important role in the intercellular communication as a mediator of RNA, protein, and lipids, therefore, it can be expected to be utilized for disease prognosis and treatment. However, the separation of lipoproteins and exosomes from blood has not been studied extensively. Field-flow fractionation (FFF) is capable of separating sample components from nano to micron size. In this study, lipoproteins and exosomes from blood plasma samples were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) using field programming and detected by UV spectrophotometer (UV) and multi-angle light scattering (MALS). After separation and fractionation by FI-AF4, lipoproteins and exosomes were confirmed by Western blot and transmission electron microscope (TEM).

Poster Presentation : **ANAL.P-334**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Analysis of characteristic serum lipids of post-hepatectomy liver failure from partially hepatectomized swine using nanoflow UHPLC-ESI-MS/MS

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Department of Chemistry, Yonsei University, Korea

Since liver possesses the big capacity to regenerate, hepatectomy is a common treatment for the disease like hepatocellular carcinoma. However, liver resections are complex operations and have a risk of complication. Especially, post-hepatectomy liver failure (PHLF) which is a liver failure after operation is one of the most serious complications and a big part of the reason of death. Liver has an important role in lipid metabolism. Therefore if liver doesn't function properly, the homeostasis of lipids might be failed. In this study, the changes of lipid profiles of swine serums were observed depending on rate of hepatectomy and time after operation using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS) to give more accurate insight into PHLF. The swines were divided into fake operation group (sham, n=6), 70% partial hepatectomy group (70% PHx, n=7), and 90% partial hepatectomy group (90% PHx, n=7). The serums were collected before operation, and 14 hours, 30 hours, and 48 hours after operation from each groups. The extracted lipids were structurally identified based on collision-induced dissociation (CID) experiments and individual serums were quantitatively analyzed through selective reaction monitoring (SRM) mode. The identified lipids were 142 phospholipids, 23 sphingolipids, and 240 glycerolipids.

Poster Presentation : **ANAL.P-335**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Profiling of lipoproteins from postmenopausal patients with osteoporosis by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

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Pathological mechanism of osteoporosis is unknown, but osteocytes affected by oxidized lipids inside the body have been known as a major factor. Bone mineral density (BMD) reaches at a highest level in mid 30s and decreases slowly over time, meaning that symptoms are hard to be detected and already serious when found out. Lipids play important roles in signal transmission, cell formation, and various cellular processes and they are expected to be biomarkers of a number of diseases. Therefore, it is interesting to study relationships between lipids consisting lipoproteins in plasma and osteoporosis for early diagnosis. There are several studies about lipids and osteoporosis in the medical field which BMD showed a positive correlation with low-density lipoprotein (LDL) and an inverse correlation with high-density lipoprotein (HDL). However, none of them conducted quantitative and qualitative analysis at the molecular level in detail. In this study, 39 plasma samples of woman were classified into three groups of patients in which women having osteoporosis with no clinical history (n=10), women having osteoporosis with history (n=7), age-matched control (n=22). Lipoproteins were first separated by sizes using asymmetrical flow field-flow fractionation and then lipids contained in HDL and LDL were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS).

Poster Presentation : **ANAL.P-336**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Optimal purification method for expression of human melanocortin-4 receptor

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The human transmembrane protein (hTMP) is the type of integral membrane proteins and exists as a signal transduction, intercellular communication, and ion channels, etc. Thus, it has various functions in the biological membrane. In order to demonstrate the function of the transmembrane proteins, the protein should be purified to identify the structure because function is related to structure closely. However, since the transmembrane protein is most composed of hydrophobic amino acids and is surrounded by the lipid, expression and purification of transmembrane protein are not easy. The transmembrane protein, which plays a biologically important role, is associated with the onset of many diseases. If a mutation occurs in human melanocortin-4 receptor (hMC4R), one of the transmembrane proteins, cause eating disorder and obesity. Asparagine-substituted mutants in aspartic acid, the 90th amino acid in the second transmembrane protein (TM2), were found in the patients with early onset obesity. It was thought that the loss of function was caused by structural changes of hMC4R due to the D90N mutation. Therefore, we examined the structural differences between wild-type hMC4R-TM2 (wt-hMC4R-TM2) and mutant hMC4R-TM2 (m-hMC4R-TM2) after expression and purification of two proteins. In the experimental process, SDS was used as a detergent when separating proteins using FPLC to separate them from impurities using hydrophobicity of target proteins. Afterwards, purified high yield target proteins were obtained by using SDS removal method, and the final structure was confirmed by various spectroscopic methods like MS, CD, solution NMR spectroscopy, and solid-state NMR spectroscopy.

Poster Presentation : **ANAL.P-337**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Design of truncated-IK protein's derivatives that alleviate inflammation

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Rheumatoid arthritis is a chronic inflammatory disease. In Rheumatoid arthritis, activated immune cells attack the synovial membrane, cartilage and bone of the joints. So, the synovial membrane is abnormally proliferated and the bones and joints are destroyed. Although there are many causes for the disease, it is known that self-antigen recognition through abnormal MHC class II-expressing B cells excessively produces antibodies. Recent studies have shown that inhibitor K562 leukemic cell has been isolated and purified from the conditioned culture medium. This truncated IK (tIK) downregulates MHC class II on activation in inflammatory diseases. In our study, we examined the phosphorylation pattern of protein cell signaling by isolating macrophages from transgenic mice transplanted with the tIK nucleotide sequence, and found that tIK protein had the same effect as the anti-inflammatory cytokine IL-10. Therefore, we focused on the process of finding derivatives that are shorter and better anti-inflammatory than the previously reported tIK protein. We predicted the possible structure of tIK based on IL-10 through sequence homology modeling and could derive an epitope associated with anti-inflammatory activity. Based on these results, we proposed 4 anti-inflammatory peptide candidates and identified the anti-inflammatory activity through the TH17 cell differentiation test. Among them, the 18-mer peptide with anti-inflammatory activity was named tIK-YK4 and the short derivatives 9-mer and 14-mer peptides were also designed. Currently, we have successfully performed overexpression using E. coli and are optimizing the purification process. We are confirming peptide candidates using various techniques such as PAGE, CD, MASS.

Poster Presentation : **ANAL.P-338**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Headspace in-tube microextraction of chlorophenols by capillary electrophoresis-electrospray ionization-mass spectrometry

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Capillary electrophoresis/mass spectrometry (CE/MS) is a powerful analytical tool combining high performance separation of CE and information-rich MS. Headspace in-tube microextraction (HS-ITME) is a simplest possible scheme of liquid phase microextraction, providing sample cleanup and enrichment for volatile compounds. As a means of improving the power of CE/MS further, HS-ITME was in-line coupled with CE/MS. When HS-ITME was coupled with CE/electrospray (ESI)-MS, the capillary outlet is exposed to the open air and there was a problem of air plug formation due to evaporation of the run buffer in the capillary. By running a small amount of the sheath liquid during extraction, the evaporation problem was solved. Then without any physical modification of the CE/MS setup, dichlorophenols and trichlorophenols in an acidified aqueous solution were enriched into a basic acceptor plug at the entrance of the capillary. The chlorophenols were enriched about 50 times with a 5-min HS-ITME at room temperature, and successfully analyzed by CE/MS.[1] H. R. Lee, S. M. Cho, J. Kim, and D. S. Chung, *J. Chromatogr. A* (2014) 117[2] S. Terabe, *Anal. Chem.* (2004) 76[3] S. M. Cho, B. S. Park, W. S. Jung, S. W. Lee, Y. Jung, and D. S. Chung, *Talanta*. (2016) 729[4] G. Bonvin, J. Schappler and S. Rudaz, *J. Chromatogr. A* (2012)

Poster Presentation : **ANAL.P-339**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

An Synthetic Approach to Si/N-Doped Graphene Quantum Dots Nano-Architecture as anode for Li secondary batteries

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Despite the pulverization and unstable solid-electrolyte interface (SEI) challenges, silicon is yet a promising high capacity anode material because of its high gravimetric capacity (~4200 mAh/g). Advancements in nano-architecture Si electrodes still remain a challenge in achieving long cycling life. To overcome these issues, we synthesized N-doped graphene quantum dots wrapped with Si nanoparticles (50 nm) compensates the volume expansion and conductivity between neighboring nanoparticles. The introduction of few layers in graphene quantum dots favors in lithium insertion and improved the stability of SEI. This nano-architecture significantly improved the structural stability and conductivity, which could be used as anode material for lithium secondary batteries.

Poster Presentation : **ANAL.P-340**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Study of Solid Natural Organic Matter and Unprocessed Soil Fixed on a Metal Plate by Double Adhesive Tape with Laser Desorption Ionization Ultrahigh Resolution Mass Spectrometry

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Typically, extensive sample preparation procedures are required to perform analysis of natural organic matter (NOM) and soil organic matter. In this study, the solid NOM and unprocessed soil samples were fixed on a metal plate with double adhesive tape and the samples were directly analyzed by use of laser desorption ionization (LDI) coupled to ultrahigh resolution mass spectrometry (UHR-MS). LDI UHR-MS analysis was successfully performed with about 2–5 μg of solid fluvic and humic acid and 500 μg soil samples loaded on the metal plate. Most of the peaks reported in the previous study performed with LDI UHR-MS was observed and additional 2200 peaks were found by direct analysis of fluvic acids. Two unprocessed soil samples were directly analyzed with LDI UHR-MS. Poly-condensed aromatics, oxygenated poly-condensed aromatics, Lignin type molecules, and lipid molecules were mainly observed from two soil samples were most abundantly observed from soils. The data presented in this study clearly show that direct molecular level analysis can be performed on solid NOM and unprocessed soil samples with high sensitivity. Therefore, we expect that the suggested analytical method can be very useful for studies such as obtaining profiles of organic compounds in cored soil samples.

Poster Presentation : **ANAL.P-341**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

NMR-based urinary profiling reveals different metabolic patterns in focal segmental glomerulosclerosis and minimal-change disease

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Focal segmental glomerulosclerosis (FSGS) and a related disorder, minimal-change disease (MCD), are idiopathic glomerular disease related to podocytopathies. Although the renal biopsy is mandatory to confirm the diagnosis and guide therapeutic plans in patients with FSGS and MCD, biopsy is an invasive procedure affected by complications. We performed NMR-based urinary metabolic profiling analysis to investigate metabolic differences between FSGS and MCD. The PCA scatter plot showed a clear separation between FSGS and control groups. Moreover, MCD groups were slightly separated from FSGS groups. The significant metabolic alteration in FSGS and MCD groups compared to healthy control groups were related to tricarboxylic acid cycle, choline, and branched chain amino acid metabolism. Furthermore, metabolite that are significantly altered in the FSGS groups included alanine and lactate, whereas MCD groups contained 3-aminoisobutyrate. This study demonstrates that metabolic profiling is useful for understanding metabolic differences between FSGS and MCD patients, and diagnosing kidney disease.

Poster Presentation : **ANAL.P-342**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Simultaneous Determination of 39 Steroid Hormones in Human Urine Sample Using Liquid Chromatography-electrospray Tandem Mass Spectrometry

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Abnormal production or metabolism of steroid hormones are responsible for the development and prevention of endocrine diseases. Accurate quantification of steroid hormones is necessary for both research into clinical conditions as well as for diagnostic monitoring. In this research, an improved analytical method was developed using liquid chromatography-tandem mass spectrometry (LC-MS/MS) for the analysis of 39 steroid hormones including corticosteroids, progestins, estrogens, and androgens in urine sample. As a pre-treatment procedure prior to LC-MS/MS analysis, hydrolyzation of the human urine samples with β -glucuronidase and solid-phase extraction for purifying the samples was performed. Steroids were separated using Waters ACQUITY @ BEH C₁₈ column (2.1 x 100 mm, 1.7 μ m) and a mobile phase consisting of eluent A (0.01% formic acid and 1 mM ammonium formate in water) and eluent B (0.01% formic acid and 1 mM ammonium formate in methanol) with a gradient program at a flow rate of 0.4 mL/min. The [M+H]⁺, [M+NH₄]⁺ and [M+H-H₂O]⁺ ions were used as precursor ions to detect endogenous steroid hormones in MS. All steroids were monitored in multiple reaction monitoring (MRM) mode within 30.0 min by tandem mass spectrometry (MS/MS) with electrospray ionization in positive mode. The linearity of this method was over 0.991. The limits of detection at signal to noise (S/N) ratio of 3 were 0.1 ~ 300 ng/L. The coefficients of variation were in the range of 2 -25% for within-day variation and 2 -25% for day-to-day variation, respectively. The present method could be applied to clinical research such as diagnosis, monitoring, and biomedical investigations.

Poster Presentation : **ANAL.P-343**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of a multielement quantitation method from whole blood samples by ICP DRC MS

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There are several attempts to assess all the environmental exposures of an individual and to reveal how the measured exposures affect to human health. Whole blood samples are one of the most widely used biomatrices for evaluating exposures due to their relatively easy accessibility. There have been many studies which tried to quantify elements from whole blood samples. Most of these studies focused on toxic heavy metals. For example, the US CDC laboratory manual published in 2014 described a method for quantitation of five toxic elements -cadmium, lead, manganese, mercury, and selenium- from whole blood samples. In this study, based on the US CDC laboratory manual, we tried to develop a multielement analysis method with whole blood samples that can cover up to about 15 elements including toxic heavy metals. To achieve this, we employed an efficient inductively coupled plasma (ICP) dynamic reaction cell (DRC) mass spectrometry (MS) platform with various cell gases. We also evaluated various sample preparation conditions and analysis parameters such as dilution factors, diluent compositions, cell gases, and cleaning procedures. In this presentation, we report the current progress in this development.

Poster Presentation : **ANAL.P-344**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of a ganglioside profiling method by using a reversed phase liquid chromatography/mass spectrometry (RPLC/MS) platform

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Gangliosides are acidic glycosphingolipids which contain sugar chains with a variety of sialic acid residues. Gangliosides have several structural isomers of which glycan structures vary. However, most of reported reversed phase liquid chromatography/mass spectrometry (RPLC/MS) platforms could not separate these structural isomers. Recently, we have developed an RPLC method that could effectively separate the ganglioside isomers with a C18 column and an ammonium bicarbonate additive. In our previous study, the optimal salt condition which can give complete ganglioside isomer separation while maintaining high sensitivity was suggested. In addition, with an optimized RPLC/MS condition, we successfully profiled total gangliosides present in porcine brains with clear isomer differentiation. In this study, we further optimized our method by evaluating the limits of detection (LODs) of the major gangliosides, peak capacity, peak resolution, and so on.

Poster Presentation : **ANAL.P-345**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Hypersensitive Cancer Immunosensor Based on One-Shot Dual Signal Detection on Nano-patterned Biochip

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Three-dimensional enhanced dark-field super-resolution microscopy (3D EDF-SRM) based on hypersensitive one-shot dual signal detection was developed for immunoassay of TNF- α as a cancer biomarker. The 3D EDF-SRM is equipped with a dual view and a digital single-reflex (DSLR) camera, enabling dual signal detection which was both quantifiable and qualitatively. The standard TNF- α was quantitatively analyzed by measuring the scattering signals of 80 nm silver nanotag on an array chip with 100 nm gold spot. The localization precision in nanotag on the gold spot narrowed to $S/N = 3$) with a wide dynamic detection range of zM-pM. In addition, a recovery greater than 98% was achieved by spiking standard TNF- α into human serum samples.

Poster Presentation : **ANAL.P-346**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Accurate determination of total arsenic in rice considering arsenic species

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Accurate determination of arsenic in a sample has been important because the toxicity related to the arsenic element has been widely known. In particular, arsenic species must be well considered because their toxicity varies according to chemical form. If the total arsenic in a sample is in trace level below the allowance maximum of any arsenic species, the quantitation of total arsenic might be satisfactory. In general, for the quantitation of total arsenic in a sample, arsenic species in a sample have been not considered at all. The standard solution of total arsenic has been made by As⁵⁺ standard solution. It might be good for the sample which its major species are As⁵⁺. But, if the major species of arsenic in a sample are different from As⁵⁺, the standard arsenic species for calibration curve must be deeply considered. This study showed the amount of total arsenic in a sample could be falsely obtained by the standard solution of different arsenic species. The standard arsenic species used in this study were As³⁺, As⁵⁺, MMA, DMA and AsB. Total arsenic was analyzed in rice using various methods including standard addition method and internal standard method. Ge, In, Rh, Te and Se as internal standards were also investigated for the determination of total As in rice. The best internal standard for total arsenic in rice was Te.

Poster Presentation : **ANAL.P-347**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A study on the determination of inorganic arsenic by solid phase extraction and laser ablation inductively coupled plasma mass spectrometry

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The toxicity and chemical properties of arsenic depend on the concentration and chemical structure present in the natural environment. Inorganic arsenic is more toxic than organic arsenic, thus the accurate determination of inorganic arsenic in various samples is needed. IC-ICP-MS (Ion Chromatography-Inductively Coupled Plasma-Mass Spectrometry) is the current method for quantitative and qualitative determination of arsenic. However, the method has disadvantage of expensive and complex instrument, and elaborate sample preparation. In this study, inorganic arsenic species were separated using a membrane filter disk in the SPE (Solid Phase Extraction) method, then determined by LIBS (Laser Induced Breakdown Spectroscopy) and LA-ICP-MS (Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry). The detection limit of inorganic arsenic is 10 mg/kg by the SPE membrane filter with LIBS. The detection limit of inorganic arsenic was 1.0 $\mu\text{g}/\text{kg}$ by LA-ICP-MS. The pH value of the sample was adjusted to 4 using ammonium hydroxide and phosphoric acid for the efficient separation of inorganic arsenic species. The linear dynamic range was from 1 to 1000 $\mu\text{g}/\text{kg}$ by LA-ICP-MS, and the correlation coefficient was 0.9997. A new method using solid phase extraction and LA-ICP-MS was a accurate and sensitive method for quantitative analysis of inorganic arsenic in a sample.

Poster Presentation : **ANAL.P-348**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A simple laser-induced breakdown spectroscopy analysis method for Mg and Ca in edible salts: Sample surface height optimization and intensity normalization

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Feasibility of a simple laser-induced breakdown spectroscopy (LIBS) instrument has been investigated for analysis of Mg and Ca in edible salts. The LIBS instrument was assembled with a compact low-power diode-pumped solid-state laser and a non-gated handheld spectrometer. A simple sampling process, called a dip-and-dry method, was employed for on-site application; a piece of filter paper was dipped in aqueous solution of the sample salt and dried to be analyzed by LIBS. The analytical performance could be significantly improved by (i) optimization of the sample surface height during laser ablation and (ii) normalization of the analyte line intensities using the Na I line at 616 nm as a reference signal. For commercially available salt products, the Mg II and Ca I line intensities could be well correlated with the concentrations of Mg and Ca determined by inductively coupled plasma- optical emission spectroscopy. Our results indicate that the combination of a compact low-cost LIBS device and the simple sampling method is promising as an on-site salt quality monitoring methodology.

Poster Presentation : **ANAL.P-349**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

The role of electrophilicity with substituted para-thiophenols in Surface-Enhanced Raman Scattering

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Surface-Enhanced Raman Scattering (SERS) is considered an important analytical technique that has two main mechanisms : the electromagnetic effect related with the localized surface plasmon resonance (LSPR) of nanoparticles and the chemical effect connected with charge-transfer between nanoparticles and probe molecules. In chemical effect, the probe molecules play an main role via the chemical bonding with nanoparticles and there is much potential to find unrevealed regions to elucidate SERS mechanism completely. To understand the relationship between the electrophilicity of molecules and SERS enhancement focused on the chemical effect, para-substituted thiophenols derivatives with strong gold-sulfur interaction and gold nanorods (AuNRs) on resonance condition are chosen. We study SERS behaviors following the electrophilicity of substituent, such as electron withdrawing group (EWG) and electron donating group (EDG), in self-assembly monolayers (SAMs) system and reveal that stronger EWG groups show higher enhancement supporting our assumption that EWG propably promotes a charge-transfer in SERS.

Poster Presentation : **ANAL.P-350**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

An Analytical Method for Characterizing Naturally Occurring Compounds in Plants

Su-Kyung Moon, Youjin Seo*

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Naturally sourced chemicals produced by plants represent a viable source for compounds targeting various diseases and are widely used in products such as cosmetics, vitamins, and drugs. Sourcing these compounds relies on both robust extraction methods and accurate, reliable, scientific assays evaluating their purity, effectiveness, and toxicity. Herein, we report our assay aimed at measuring the compounds, chicoric acid and chrysophanol each derived from taraxacum officinale and cassis seed, respectively. Both these naturally occurring compounds have pivotal roles as antioxidants and are implicated in immunological disorders and atopic dermatitis. We developed an analytical method using a HPLC-UV platform assessing system suitability, linearity, specificity, accuracy, precision, homogeneity and carry-over. Our method accurately measured both compounds. In addition, our results matched the acceptance requirement of validation criteria established by ICH. This method provides a means to adhere to established guidelines and to levels of naturally occurring compounds derived from plants.

Poster Presentation : **ANAL.P-351**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Catalytic tendency analysis of SnO₂ Nanoparticles by doping of transition metal: Cr, Mn, Fe, and Co.

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Transition metal doped Sb@SnO₂ nanoparticles (TM-Sb@SnO₂) were synthesized to enhance a catalytic effect of SnO₂ which can be used for detecting Cys. As abnormal level of L-cysteine (Cys) can make some obstacles in metabolism, the detection of Cys is important in the field of diagnostics. We assess some information about size distributions, shapes of particles, and formation of single-phase by using surface analysis technique, such as transmission electron microscopy (TEM), X-ray diffraction (XRD), scanning transmission X-ray microscopy (STXM), and high-resolution photoemission spectroscopy (HRPES). Then TM-Sb@SnO₂ were evaluated catalytic effects by measuring photocatalytic oxidation and electrochemical oxidation of Cys. Through the spectral analysis, we found that the Cr- and Mn-doped SnO₂ nanoparticles exhibit enhanced catalytic activities, which according to the various surface analyses were due to the effect of the sizes of the particles and electronegativity differences between the dopant metal and SnO₂.

Poster Presentation : **ANAL.P-352**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Plasmonic sensing of biotin-BSA proteins by chemical interface damping of single gold nanorods.

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Chemical interface damping (CID) is one of the main decay processes that result in the broadening of the homogeneous localized surface plasmon resonance (LSPR) linewidth in plasmonic gold nanoparticles. However, it is the most poorly understood damping mechanism in gold nanoparticles. Herein, to better understand CID, we performed scanning electron microscopy (SEM) correlated dark-field (DF) scattering studies of single gold nanorods (AuNRs). First, we examined size-dependent broadening of the homogeneous LSPR linewidth in single AuNRs with three different aspect ratios (ARs) at a fixed diameter of 25 nm. The LSPR linewidth increased with decreasing the AR of single AuNRs because of the reduced average distance of hot electrons to the surface. Second, we examined the effect of adsorbate thiol molecules on the homogeneous LSPR linewidth in single AuNRs. The LSPR linewidth was broadened with increasing the carbon chain length of 1-alkanethiol. Third, we investigated the effect of refractive index variation of the surrounding medium on the LSPR linewidth in single AuNRs of three different sizes. The LSPR linewidth remained almost constant while increasing the dielectric constant of the medium. Last, we confirmed that CID-based biosensors can be used to detect real biological molecules such as bovine serum albumin (BSA) conjugated with biotin.

Poster Presentation : **ANAL.P-353**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Refractive Index Sensitivity of Localized Surface Plasmon Resonance Inflection Points in Single Gold Nanoparticles with Different Shapes

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Plasmonic gold nanoparticles exhibit unique size- and shape-dependent optical properties, which is caused by the localized surface plasmon resonance (LSPR) collective oscillation of conduction electrons in gold with the incident light. In this study, we investigated the medium refractive index (RI)-dependent optical properties and LSPR sensitivity of single gold nanocubes (AuNCs) and gold nanospheres (AuNSs) of similar size (50 nm) under dark-field (DF) microscopy at the single particle level. We found that AuNCs with vertices have higher sensitivity to the medium RI than spherical AuNSs. Furthermore, the LSPR inflection point (IF) at the longer wavelength showed higher RI sensitivity in single particle scattering spectra. Therefore, we provide a deeper insight into the shape-dependent optical properties and RI sensitivity of LSPR IFs at single particle level, which can be beneficial and helpful for their uses in the development of sensitive biosensors.

Poster Presentation : **ANAL.P-354**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Inhibition mechanism of human serum albumin in alpha-synuclein aggregation

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Alpha-synuclein, one of amyloid proteins that are related to the pathology of alpha-synucleinopathies (e.g. Parkinson's disease, dementia with Lewy bodies, and multiple system atrophies), self-assembles to fibrillar aggregates toxic to neuronal cells. Interestingly, the formation of alpha-synuclein aggregates is not common in human organs except for brains. As one of hypothesis, molecular interaction with plasma proteins in human fluids has been suggested to disrupt protein-protein interactions of alpha-synuclein. Human serum albumin is the most abundant protein in human fluid and is known to suppress the self-assembly of amyloid-beta peptide. Thus, human serum albumin is expected to modulate the self-assembly of alpha-synuclein. In this poster presentation, I will discuss the molecular interaction between alpha-synuclein and human serum albumin. Using multiple biophysical approaches, I have characterized that electrostatic interaction of alpha-synuclein and human serum albumin plays a crucial role in suppressing the aggregation of alpha-synuclein.

Poster Presentation : **ANAL.P-355**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

The synthesis of the Ru(dia-py)₂ Cl₂ for glucose determination with glucose dehydrogenase

Ryang Hyeon Kim, Tae-Won Seo¹, Won-Yong Jeon*, Young Bong Choi*, Hyug-Han Kim*

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The Ru(NH₃)₆ mediator has been used for transfer the electron in electrochemical glucose sensor. However, the Ru(NH₃)₆ mediator is not reacting with glucose dehydrogenase (GDH). In this study, we synthesized new Ru(dia-py)₂ Cl₂ mediator for the reaction with GDH. This is a second-generation sensor using a mediator that measures the amount of hydrogen peroxide in the first-generation sensor and improves the measurement error due to the oxygen concentration in the body to help redox. In addition, the mediator mediates the electron transfer from the active site of the enzyme and the electrode, and has high selectivity and sensitivity, which helps to detect glucose. Ru(dia-py)₂ Cl₂ was synthesized by using RuCl₃ and 4,4'-Diamino-2,2'-bipyridine. The Cyclic Voltammetry (CV) was used as an electrochemical method to check for their electrochemical properties. It was found that the combined mediators and GDH are physically fixed to the electrodes to enable concentration analysis using an electrochemical method of glucose. The modified electrodes were physically immobilized on the electrode, and confirmed that glucose concentration were analyzed by CV.

Poster Presentation : **ANAL.P-356**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

The electrochemical catalytic reaction depending on the different molecular weight with PAA-PVI-osmium complex and glucose dehydrogenase

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Screen printed carbon electrodes(SPCEs) is widely known as electrochemical reaction sensing platforms due to their simple fabrication in terms of compositions and relatively low cost of production. The Poly(acryl amide)-Poly(vinyl imidazole)(PAA-PVI)-osmium complex mediator was employed onto SPCEs with glucose dehydrogenase (GDH), which is to oxidase the glucose. The different molecular weight in redox polymer was controlled by initiator and catalyst, and then it was identified by gel permeation chromatography (GPC). The PAA-PVI-osmium complexes were synthesized by the coordinating pyridine group having different functional group at 4-position with osmium compounds. The electrochemical catalytic reaction effect depending on molecular weight was measured by cyclic voltammetry with modified SPCEs. The electrical currents by the different molecular weight were shown with a good linear response with glucose concentrations with GDH. These results can help to develop in the medical diagnosis field and electrochemical biosensor.

Poster Presentation : **ANAL.P-357**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical biosensor for detection of uric acid using polydopamine@multi-walled carbon nanotubes.

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Department of Chemistry, Dankook University, Korea

The uric acid has known as the bio-marker for early detection of the gout. The electrochemical biosensing has been applied for quantitative analysis of uric acid. The Polydopamine (PDA) is the good candidate for hydrophilic functionalization of the multi-walled carbon nanotubes (MWCNTs). The PDA coated MWCNTs (PDA@MWCNT) were adsorbed onto the indium tin oxide (ITO) electrode with uricase enzyme. Polyacrylic acid(PAA) was additionally coated to block the interfering substances. The modified electrodes were used to quantitatively analyze the uric acid by measuring with Cyclic Voltammetry(CV). Measurement of ascorbic acid(AA), dopamine(DA), and glucose, which are interference substrates in the human body, was shown no interference effect. The calibration curve was drawn using the uric acid of various concentrations(0.1, 0.5, 1.0, 1.5, 2.5, 5.0mM) as the above prepared electrode, and it was found that $R^2 = 0.99$ showed good linearity. Finally, this study can be used for early diagnosis in the health care fields.

Poster Presentation : **ANAL.P-358**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Biosensor application of the "Ru(ter-py)Cl₃ " mediator for glucose determination

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The biosensor that measure the glucose level through electrochemical methods are excellent device. However, conventional glucose sensors has measured the concentration of the glucose through GOX, which is affected by the concentration of oxygen in the blood. As a result, GOX based glucose sensor has been showed a little bit error due to diferrent oxygen concentration. To solve these drawbacks, we have studied glucose sensor based on GDH. However, since existing electron transfer mediators that respond to GOX not respond to GDH, a new electron transfer mediator has to be made in order to develop a glucose sensor using GDH. In this study, the ligand of the 2,2'-6',2"-terpyridine was coordinated into the center of the RuCl₃ . And it was confirmed that the intensity of the electric signal according to the concentration of glucose by cyclic voltammetry (CV) and it shown good linearity.

Poster Presentation : **ANAL.P-359**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Effect of adsorbate electrophilicity and sharp tips on single gold nanobipyramids.

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Gold nanoparticles behave as strong absorbers and scatterers because of localized surface plasmon resonance (LSPR) which is coherent oscillation of conduction electrons at the surface of plasmonic nanoparticle stimulated by the electromagnetic field of incident light. The LSPR peak shift is caused by changes in the medium dielectric constant. However, our understanding of the effects of electrophilicity of thiol molecules adsorbed on gold nanoparticle surfaces is still unsatisfied. In this study, we present dark-field (DF) scattering studies on electrophilicity effect of adsorbate molecules with real time measurement at the single particle level. We found that LSPR wavelength of the gold nanobipyramids (AuBPs) was red-shifted as thiol molecules were adsorbed onto their surface. The electrophilicity of adsorbate molecules was strongly affected to degree of red-shift. Furthermore, the red shift of LSPR wavelength of single AuBPs were rapidly saturated in real-time measurement. This result indicate that AuBPs are highly sensitive to thiol molecules because of the sharp tips and can be used to develop highly sensitive LSPR biosensors.

Poster Presentation : **ANAL.P-360**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

The Effect of Electrophilicity of Thiol Molecules in Chemical Interface Damping of Single Triangular Gold Nanoplates

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Plasmonic nanoparticles have been extensively studied for various applications such as photocatalyst, bio-sensor, orientation probe, photothermal cancer therapy etc. This is because they exhibit unique size and shape dependent optical properties resulted from the localized surface plasmon resonance (LSPR) effect. The LSPR is vibration of free electrons in the conduction band induced by interaction with an electromagnetic field. Recently, two-dimensional (2D) triangular gold nanoplates (AuNPs) are of great interest in many applications such as nanocatalysis and biosensors due to their characteristic LSPR property caused by triangular shape. However, chemical interface damping in single AuNPs at the single particle level has not yet been studied so far. In this study, we characterized the optical properties of single AuNPs and thiolate effect under dark-field (DF) microscopy. The LSPR damping was observed for single thiol-capped AuNPs due to chemical interface damping effect on their surface under single particle scattering spectroscopy. Furthermore, thiol molecules with strong electron withdrawing group (EWG) was compared to strong electron donating group (EDG) on chemical interface damping in single AuNPs. Therefore, we found the potential use of single AuNPs as plasmonic biosensors using this chemical interface damping.

Poster Presentation : **ANAL.P-361**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A SERS-based microdroplet chip for simultaneous immunoassays of dual prostate cancer markers

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For the fast and accurate detection of prostate cancer markers, a novel surface-enhanced Raman scattering (SERS)-based microfluidic chip was developed for the simultaneous detection of free prostate-specific antigen (f-PSA) and total PSA (t-PSA) markers. In this study, we described a fully automatic droplet-based microfluidic platform for the rapid and sensitive detection of f-PSA and t-PSA. The device was composed of three compartments: mixing and reaction, auto separation, and SERS detections. Sandwich immunoassays for f-PSA and t-PSA biomarkers were performed using sequential microdroplets to avoid tedious washing steps. Raman signals of sequential droplets including supernatant solutions were measured for the quantitative analysis of the PSA markers. The results showed a good linear response for both PSA markers in the range from 0.05 to 100 ng mL⁻¹. The limits of detection were estimated to be below 0.1 ng mL⁻¹ for both the f-PSA and t-PSA. This low LOD level demonstrates that the detection limit of our SERS-based microfluidic immunoassay is much lower than the clinical threshold. Therefore, our proposed method is a very promising clinical tool for the PSA-based screening test of prostate cancer. References 1.R. Gao, Z. Cheng, X. Wang, L. Yu, Z. Guo, G. Zhao, J. Choo, *Biosens. Bioelectron.*, 119, 126 (2018). 2.Z. Cheng, N. Choi, R. Wang, S. Lee, K.C. Moon, S.-Y. Yoon, L. Chen, J. Choo, *ACS Nano*, 11, 4926 (2017). Keywords: SERS, microdroplet device, PSA, multiplex immunoassays

Poster Presentation : **ANAL.P-362**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Support Effect of Plasmonic Nanoparticles on Carbon Nanotubes at Single-molecule Level

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Supported catalysts were synthesized with gold nanoparticles deposited on the outer surface (Au/CNTs-out) and inner surface (Au/CNTs-in) of CNTs by wet chemistry method. Single-molecule nanocatalysis measurements were carried out using a lab-built prism-type total internal reflection fluorescence microscope (TIRFM) by detecting the fluorescence from the reduction reaction catalyzed over Au/CNTs-out and Au/CNTs-in. The results indicated the support effect of CNTs in both product formation process and product dissociation process. For the product formation process, Au/CNTs-out showed higher catalytic activity than Au/CNTs-in because gold nanoparticles on the exterior of CNTs have relatively enriched electrons compared to those on the interior walls. For the product dissociation process, Au/CNTs-out exhibited the faster product molecules dissociation rate than Au/CNTs-in. Moreover, same dissociation pathway was observed. Product molecules on both Au/CNTs-out and Au/CNTs-in preferred the reactant-assisted dissociation pathway. Our research advances the traditional single-molecule method to provide insights into the supported catalysts.

Poster Presentation : **ANAL.P-363**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis, dispersion and tribological performance of alkyl functionalized graphene oxide as an oil lubricant additive

Jong Seok Han, Jin-Yeong Choi, Chang-Seop Lee*

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Graphene has been reported as an excellent lubricant additive for reducing adhesion and friction, when coated on the various surfaces as an atomically thin material with low surface energy. Various methods have been proposed to enhance the physical properties of GO by its reduction, because it is difficult to apply GO to hydrophobic lubricant due to the large numbers of oxygen functional groups and the remarkably poor physical properties. To solve this problem, many attempts have been made to transform graphene into covalent bonds or noncovalent bonds. We have developed graphene oxide (GO) grafted with long alkyl chains to improve dispersion in oil-base lubricant as largely enhanced lipophilicity. Alkyl functionalized GO is synthesized by reacting NH₂-GO with hexyl chloride, dodecyl chloride, hexadecyl chloride in ethanol under reflux, then 1.0x10⁻³ wt% of alkyl functionalized GO are added into the base oil (PAG oil) and oil containing WS₂ and also ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene are investigated by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), and Scanning electron microscope (SEM). The tribological tests are performed with a tribometer via ball-on-disk test mode.

Poster Presentation : **ANAL.P-364**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Binder-free carbon nanotube/Si composite films as an advanced anode for lithium ion batteries

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Carbon nanotube/Si composite binder-free electrode is used anode for lithium ion batteries (LIBs). We report the fabrication of binder-free anodes for lithium-ion batteries based on CNT/silicon composite films on-demand designed and composite film is designed and produced by ultrasonic fracture cutting the carbon nanotubes. A mixture of multi-wall carbon nanotubes and silicon powder was dispersed in NMP for ultrasonic exfoliation, and then the resulting dispersion was subjected to ultracentrifugation to remove the thick flakes and the un-exfoliated carbon nanotubes. The supernatant after centrifugation is collected for vacuum filtration, and 1 L of ethanol is added to the suction bottle in batches to obtain a composite film. The physicochemical properties were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. The electrochemical properties were also investigated by Galvanostatic charge-discharge and Electrochemical Impedance Spectra (EIS).

Poster Presentation : **ANAL.P-365**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Comparative Analysis of Lectin based Glycoproteomics and Triglyceride and Glucose (TyG) Index between Elderly Yoga Groups

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We had already investigated the efficacy of elderly yoga by identifying and comparing the glycoproteins in human plasma. This study focused on comparing the efficacy of yoga with the change of Triglyceride and Glucose (TyG) Index from Advanced level group and Beginner level group. The TyG Index can predict diabetes with simple calculation. The glycoproteins from the yoga participants' plasma are affinity selected using self-packed *Lycopersicon esculentum* lectin (LEL) columns. After that, peptides from affinity selected proteins were deglycosylated with PNGase F and identified with nLC-MS/MS. The results show that the number of plasma glycoproteins in Advanced level group is less than that in Beginner's group, demonstrating an inverse correlation between number of plasma glycoproteins and yoga experience. Additionally, the decrease of TyG Index in Advanced level group is higher than Beginner level group, which is similar to the tendency of glycoprotein change between elderly healthy yoga groups.

Poster Presentation : ANAL.P-366

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Comparison of optical purity of 2,2,2-trifluoro-1-(9-anthryl)ethanol and some chiral compounds by NMR spectroscopy and high performance liquid chromatography

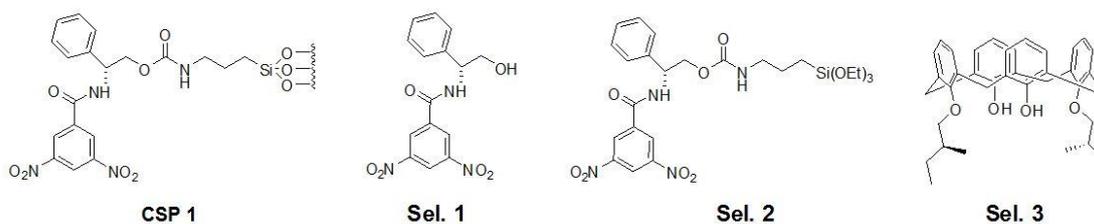
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N-3,5-dinitrobenzoyl-(*R*)-phenylglycinol and its silylation product were used as an HPLC chiral stationary phase(CSP 1) for the resolution of racemic analytes including 2,2,2-trifluoro-1-(9-anthryl)ethanol(A).¹ Due to the low selectivity($\alpha=1.16$) of A on CSP 1, determination of optical purity of A could not check correctly. In this study, we determined the optical purity of A and some chiral compounds using NMR spectroscopy and HPLC. Chiral selectors (Sel 1, Sel 2, Sel 3) used for NMR spectroscopy are shown below.

[1]. Jae Jeong Ryoo. et al. Chirality 28, 186–191 (2016)



Poster Presentation : **ANAL.P-367**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical Detection of *Aspergillus niger* by Microgap Device

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Aspergillus niger (*A. niger*), called black mold, is one of the most common fungi. *A. niger* can cause plant disease in vegetables and fruits such as onions, peanuts, grapes, and many others. We detected *A. niger* using electrochemical sensor that is based on interdigitated microelectrodes. When micro-sized fungi were located on the micro gap region by antibodies immobilized on the SiO₂ surface between electrodes, the redox signal of ferricyanide was decreased due to the hindrance of the electron transport. The decrement of redox signal was influenced by the concentration of fungi. By using this method, it was able to quantify concentration of fungi and the sensor showed remarkable selectivity compared to that of *E. coli*.

Poster Presentation : **ANAL.P-368**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Effects of *Ecklonia cava* extract intake on endogenous and exogenous metabolites in human urine

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Ecklonia cava is a sort of brown algae native to Korea and Japan, containing unique polyphenols referred to as phlorotannins. Recently, several studies have been examined the effect of phlorotannins, which reduces body fat and improves cardiovascular function. However, there are few metabolic studies relevant to those effects in human model. In this study, we performed a comprehensive metabolomics analysis of urine from males and females with a BMI over 25kg/m² and under 30kg/m² using ultra-performance liquid chromatography quadruple time-of-flight mass spectrometry (UPLC-Q-TOF-MS) to investigate effects of *Ecklonia cava* extract (Seapolynol) intake on the exogenous and endogenous metabolites. Statistical analysis were performed with correlation analysis and Hierarchical clustering analysis. We found that several endogenous and exogenous metabolites were significantly associated with Seapolynol intake, such as sulfonic acid, organic acid, xanthine and flavonoid glycoside. Especially, the levels of methyl xanthine and methyl uric acid were increased, whereas flavonoid glycoside was decreased in Seapolynol group. This study demonstrates that UPLC / MS based urine metabolic approach can be used to investigate the metabolic effects of Seapolynol intake and provide the insight for metabolism.

Poster Presentation : **ANAL.P-369**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Quickly probing the internal chemicals of a container using SORS fiber optic probes

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Technology to investigate hidden chemical information of components inside container is attracted attention in airport security, pharmaceutical process, chemical synthesis process and medical field. This technology requires non-destructive and rapid identification of the internal components in the container. Spatially offset Raman spectroscopy (SORS) is a potential candidate for investigating the chemical information of hidden substance in a container. SORS is a method of measuring Raman signal along the distance between the laser irradiation point and the detection point. The Raman signal generated by the penetration of the laser into the inside is observed to be relatively stronger as the distance increases. Therefore, SORS not only can quickly and nondestructively identify the structure of a chemicals, but it is also useful for detecting hidden substances inside containers. In this study, we fabricated SORS fiber optic probes to facilitate SORS measurements. The SORS fiber optic probe is designed so that detection point is located at offset of 5 and 10mm on both sides from the center laser is irradiated. The Raman signal obtained from the SORS fiber optic probes was subjected to internal reference subtraction to remove the Raman signal of the container. We have used a fiber optic probe to measure and database various chemicals in the container. SORS measurements using fiber optic probes have proven to be non-destructive and quick to measure the material in the container.

Poster Presentation : **ANAL.P-370**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Determination of vapor pressure for melt-cast explosives

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Agency for Defense Development, Korea

Melt-cast explosives not like common solid molecular explosives could be instantly loaded in the warhead by melting and casting without any other processes. So melt-cast explosives are still important because of their instant productivity. For melt-cast explosives, vapor pressure is one of the important properties. Because if vapor pressure is relatively high in the mid-temperature range, it would be really harmful for melting and loading processes. Here in, we describe convenient simple method for determination of vapor pressure using TGA (ThermoGravimetric Analysis) measurements.

Poster Presentation : **ANAL.P-371**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Highly sensitive molecular diagnostics using SERS-PCR

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Recently, quantitative real-time PCR (QPCR) have been extensively used for the diagnosis of a wide range of infectious diseases. This technique found valuable clinical application in the diagnosis of viral diseases. However, QPCR suffers from several problems including time-consuming process and high fluorescent background signal. In the present work, we developed a novel molecular diagnostic method using SERS-PCR for the sensitive and specific detection of target genes. Due to the characteristics of amplifying Raman signals by factors up to 10-14 orders of magnitude and unique molecular fingerprinting information, surface-enhanced Raman scattering (SERS)-based biosensors provide ultrahigh sensitivity and have more advantages over the fluorescent detection method. In the present study, we employed an asymmetric-PCR to amplify the target gene in a short time, and then a SERS detection technique has been used for its highly sensitive detection. By combining the PCR and SERS as a detection tool, it would prove to be effective for the rapid and sensitive detection of a low concentration of target. References 1.Kneipp, K., Wang, Y., Kneipp, H., Perelman, L. T., & Itzkan, I, Phys. Rev. Lett. 78, 1667 (1997).2.Wu, Y., Jiang, T., Wu, Z., & Yu, R, Biosens. Bioelectron, 99, 646-652 (2018).Keywords: SERS-PCR, Pseudomonas aeruginosa, Ratiometric gene detection, molecular diagnostics

Poster Presentation : **ANAL.P-372**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Resonance Raman Analysis of Korean Traditional & Modern Pigment

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In the analysis of art and cultural heritage, methods that do not directly damage the analyte are needed. Raman spectroscopy, which analyze the molecular vibration information by investigating the inelastic scattering light generated by the laser irradiated on the analyte, can find the molecular composition, physical structure and chemical bonding of the analyte. With this property, Raman spectroscopy is a non-destructive and effective spectroscopic instrument when examining the chemical composition of the analyte. . However, strong fluorescence of pigments interferes with the measurement of weak Raman signals. By using multiple wavelength lasers in Resonance Raman scattering (RRS), we could increase the efficiency of Raman signal while reducing the fluorescence of Korean pigments. Depending on the electronic state of the pigment, the specific excitation wavelength not only suppresses fluorescence but also increases the Raman signal (RRS). Therefore, selection of the excitation wavelength is the most basic step in the Raman analysis of art and archeology, and the next step is to consider the color, chemical structure, and resonance Raman scattering efficiency. In this research, we investigated the electronic absorption / emission spectrum and Raman spectrum of various traditions and modern Korean pigments. Resonance and non-resonance Raman spectra were obtained at six excitation wavelengths whose intensities were inferred from the state of the electrons. And we are currently building a library matching algorithm based on multicolor Raman spectroscopy library of Korean pigment, chemical measurement and machine learning.

Poster Presentation : **ANAL.P-373**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Disposable HPLC micro-column with a welded stainless-steel frit at the column outlet and a silver cemented frit at the column inlet

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In this study, we have developed a disposable microcolumn with a welded metal frit and a silver cement frit. First, one end of 30 cm glass-lined stainless-steel tubing (1.6 mm od, and 0.5 mm id) was welded with a stainless-steel screen frit of 1.6 mm diameter using a micro-welding machine. Next, the column was connected to a slurry packer and packed with C18 bound partially sub-2 μm silica monolith particles. Next, a silver cement frit was made inside the column by injecting the reaction mixture into the packed column. Silver is reduced on the particle surface and in an empty space among the particles, forming a solid silver network structure at the column inlet area. This silver cemented frit can hold the stationary phase inside the column even at a high flow rate. The column was tested for separation of a test mix composed of phenol, acetophenone, 4-methyl-2-nitroaniline, benzene and toluene. The chromatographic performance of this column (with a metal welded frit and a silver cemented frit) was compared with another column (same dimension) with two screen frits packed with the same stationary phase. The columns of a welded frit and a silver cemented frits showed ca. 15 % better separation efficiency (number of theoretical plates) than those of two screen frits. This study shows a promising vision for realization of disposable micro-columns.

Poster Presentation : **ANAL.P-374**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of solid phase extraction cartridge filled with ground organic monolith particles

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In this study, a stationary phase based on organic monolith particles has been developed for solid phase extraction (SPE). Firstly, a soft organic monolith was prepared by heating the mixture of methyl methacrylate (MMA), trimethylolpropane trimethacrylate (TPTM), polyethyleneglycol (PEG 100,000), azobisisobutyronitrile (AIBN) and n-butanol. The soft solid bulk monolith was smashed into particles. The organic monolith particles were washed, dried and the very fine particles and residual chemicals were removed using cellulose thimble filters installed in a soxhlet apparatus. The final product was packed in a 3 ml SPE cartridge and used for solid phase extraction of dialkyl phthalates. An aqueous sample solution of 10 mL was prepared by dissolving dibutyl phthalate, dicyclohexyl phthalate and dioctyl phthalate at a concentration of 5 ppm each, and passed through the cartridge. The captured analytes were recovered with acetone and ethylacetate as the releasing solvents. The recovery was about 90% for all analytes.

Poster Presentation : **ANAL.P-375**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A facile method to fabricate multi-walled carbon nanotubes with embedded/confined metal oxide nanoparticles

TaeHyeong Kim, Seunghyun Lee*

Department of Nanochemistry, Gachon University, Korea

A facile method to fabricate multi-walled carbon nanotubes (MWCNTs) with metal oxide nanoparticles using metal hydrate as precursors has been successfully achieved via physical processes. The processes create defects on MWCNTs, in which various metal oxide nanoparticles are embedded in the wall of carbon nanotubes or forms metal oxide nanoparticles confined inside MWCNTs. In the former case, transition metal oxide nanoparticles are produced on the MWCNTs under a condition of relative low temperature and atmospheric environment. Simultaneously, the oxide nanoparticles move along the surface of MWCNTs and subsequently generate defect sites by reacting carbon and oxygen. Here, we present the evidences of defect sites produced by our processes and structural effects by different types of metal hydrates.

Poster Presentation : **ANAL.P-376**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

VX Evaporation from Soil Surface

Jun oh Lee

Agency for Defense Development, Korea

Nerve agents such as VX, Sarin(GB), and Soman(GD), have been found to be used chemical attacks in Syria. In addition, Jong-nam Kim was suspected to be killed by a lethal nerve agent VX, the most toxic nerve agents of the known chemical agents. However, there are few database on the behavior of VX in the event of evaporation on various surface. In this work, the evaporation characteristics of VX chemical agent from soil was measured under certain environmental condition. Experiments were performed in a laboratory-sized wind tunnel. The vapor was collected in the form of EMPF vapor (VX's G-analog), using thermal desorption tubes which were then analyzed by gas chromatograph. We believe that these results would be helpful to build up database of VX under a variety of condition.

Poster Presentation : **ANAL.P-377**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Measurement of Reactive Oxygen Species (ROS) using Spectrophotometry and Investigation of Cell Phototoxicity Mechanism

Hyeyoung Kim, Sujin Cho¹, Tian Tian¹, Seog Woo Rhee^{1,*}

Kongju National University, Korea

¹Department of Chemistry, Kongju National University, Korea

In this study, we measured the amount of reactive oxygen species (ROS) generated by light-sensitive materials using spectrophotometric method and investigated cell phototoxicity mechanism evaluated using 3T3 NRU test. Amiodarone HCl (AD) and chlorpromazine HCl (CP) were selected as phototoxicity standard materials. The amount of singlet oxygen species and superoxide anions generated by photoreactivity was quantitated by spectrophotometry. Based on this, the toxicity mechanism of each standard material was identified by comparing with IC50 value of 3T3 NRU Test. Based on the results of this study, it is expected that cell phototoxicity can be evaluated through in vitro experiments on materials that cause ROS by photoreaction.

Poster Presentation : **ANAL.P-378**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Solution state structure of P11 the mimetic peptide derived from IgG antigen Apo-B100 by NMR

GilHoon Kim, Hoshik Won*

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Apolipoprotein B-100, the major component of low density lipoprotein (LDL), is cholesterol-transporting lipoprotein in human plasma. Apo B-100 is responsible for the binding of LDL to the LDL receptor. Modification of lysine residues of apo B-100 by acetylation or MDA-modification prevents the binding of LDL to the LDL receptor. Modified LDL binds to the acetyl LDL receptor with high affinity that contributes to the accumulation of cholesterol in foam cells of atherosclerotic lesions. For this reason, apo B-100 has been received clinical attentions for the use of diagnosis marker of atherosclerosis. Structural studies of group A peptides P11, P25, and P74 were performed based on the previous results of ELISA (enzyme-linked immunosorbent assay) tests showing atherosclerosis-inducing immune responses for 302 peptides, 20 amino acids long partial peptides of MDA-oxidized apo B-100. Among 302 peptides, group A peptides showed high level of IgG antibody after oxidation. NMR spectra were used to determine protein structures. NMR signal assignments of peptides were made by using homonuclear 2D NMR techniques including COSY, TOCSY and NOESY. Intraresidual and interresidual NOE connectivities used for structure determination were obtained from NOESY spectra. Chemical shifts of each peaks could be obtained by peak pick function in NMRViewJ. Advanced filter and macro function of Excel were used to identify peaks out of the overlapped peaks. On the basis of these distance data from NMR spectra, distance geometry and molecular dynamic were carried out to determine tertiary structures of P11, P25, and P74. Iterative 2D NOE back-calculation and theoretical NOE spectrum generation were made to obtain the final solution-state NMR structures of peptides. Comparisons were carried out until experimental spectrum matches with theoretical 2D NOE spectrum.

Poster Presentation : **ANAL.P-379**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Solution state structure of P105, P177 the mimetic peptide derived from IgM antigen Apo-B100 by NMR

Nayoung Lee, Kyoung-Ho Park, GilHoon Kim, Hoshik Won*

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Apo B-100 is composed of 4536 amino acids that make up the major component of low density lipoprotein (LDL), is cholesterol-transporting lipoprotein in human plasma. Apo B-100 is responsible for the binding of LDL to the LDL receptor. Modification of lysine residues of apo B-100 by acetylation or MDA-modification prevents the binding of LDL to the LDL receptor. Modified LDL binds to the acetyl LDL receptor with high affinity that contributes to the accumulation of cholesterol in foam cells of atherosclerotic lesions. For this reason, apo B-100 has been received clinical attentions for the use of diagnosis marker of atherosclerosis. Structural studies of group B peptides P105, P177 were performed based on the previous results of ELISA tests showing atherosclerosis-inducing immune responses for 302 peptides (P1-P302), 20 amino acids long partial peptides of MDA-oxidized apo B-100. Among 302 peptides, P105 and P177 of group B peptides showed high level of IgM antibody after oxidation. NMR spectra were used to determine protein structures. NMR signal assignments of peptides were made by using homonuclear 2D NMR techniques including COSY, TOCSY and NOESY. Intraresidual and interresidual NOE connectivities used for structure determination were obtained from NOESY spectra. Chemical shifts of each peaks could be obtained by peak pick function in NMRViewJ. Advanced filter and macro function of Excel were used to identify peaks out of the overlapped peaks. On the basis of these distance data from NMR spectra, distance geometry and molecular dynamic were carried out to determine tertiary structures of P105 and P177. Iterative 2D NOE back-calculation and theoretical NOE spectrum generation were made to obtain the final solution-state NMR structures of peptides. Comparisons were carried out until experimental spectrum matches with theoretical 2D NOE spectrum.

Poster Presentation : **ANAL.P-380**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Quinone-based Photoinduced Molecule for Preparing Surface Patterning

Geun-Hyeok Yu, Woon-Seok Yeo*

Bioscience and Biotechnology, Bio/Molecular Informatics Center, Korea

In this poster, we report on a synthesis of the quinone-based trimethyl lock (Q-PTL) decaging molecule and its application for surface patterning. The trimethyl lock system is based on the ortho-hydroxydihydrocinnamic acid derivative that undergoes lactonization upon a reduction leading to release of a molecular moiety. Therefore, trimethyl lock system have been widely used in various ways through controlling the lactonization reactivity with enzymes, electrical potentials, and chemical/photochemical reductions. Among these, the photochemical reduction does not require any complicate reagents other than light and is relatively easy to control with very few variables by other substances. By taking advantage of these features, we introduced the photocleavable Q-PTL molecule on self-assembled monolayers (SAMs) for surface patterning. The Q-PTL molecule was synthesized to have acid functionality, which was then immobilized to monolayers by using EDC/NHS coupling reaction. The monolayers were irradiated with UV light through the patterned photomask and the photo-induced release of a molecular moiety and the resulting patterns were confirmed by matrix-assisted laser desorption/ionization time of flight mass spectrometry and fluorescence. We believe our strategy can be used in various applications requiring micropatterns of DNA, proteins, peptides, cells, and other biomolecules.

Poster Presentation : **ANAL.P-381**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Solution state structure of P102, P103 the mimetic peptide derived from IgM antigen Apo-B100 by NMR

JungEun Kim, GilHoon Kim, Kyoung-Ho Park, Hoshik Won*

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Apo B-100 is composed of 4536 amino acids that make up the major component of low density lipoprotein (LDL), is cholesterol-transporting lipoprotein in human plasma. Apo B-100 is responsible for the binding of LDL to the LDL receptor. Modification of lysine residues of apo B-100 by acetylation or MDA-modification prevents the binding of LDL to the LDL receptor. Modified LDL binds to the acetyl LDL receptor with high affinity that contributes to the accumulation of cholesterol in foam cells of atherosclerotic lesions. For this reason, apo B-100 has been received clinical attentions for the use of diagnosis marker of atherosclerosis. Structural studies of group B peptides P102 and P103 were performed based on the previous results of ELISA tests showing atherosclerosis-inducing immune responses for 302 peptides (P1-P302), 20 amino acids long partial peptides of MDA-oxidized apo B-100. Among 302 peptides, P102, P103 of group B peptides showed high level of IgM antibody after oxidation. NMR spectra were used to determine protein structures. NMR signal assignments of peptides were made by using homonuclear 2D NMR techniques including COSY, TOCSY and NOESY. Intraresidual and interresidual NOE connectivities used for structure determination were obtained from NOESY spectra. Chemical shifts of each peaks could be obtained by peak pick function in NMRViewJ. Advanced filter and macro function of Excel were used to identify peaks out of the overlapped peaks. On the basis of these distance data from NMR spectra, distance geometry and molecular dynamic were carried out to determine tertiary structures of P102 and P103. Iterative 2D NOE back-calculation and theoretical NOE spectrum generation were made to obtain the final solution-state NMR structures of peptides. Comparisons were carried out until experimental spectrum matches with theoretical 2D NOE spectrum.

Poster Presentation : **ANAL.P-382**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Investigation on the correlation between levels of glutathione and curcumin using gold nanoparticles and MALDI-TOF MS

Geon-Young Yoo, Woon-Seok Yeo*

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In this poster, we present the correlation between the curcumin level and glutathione (GSH) level in mammalian cells, which were investigated by using gold nanoparticles (AuNPs) and matrix-assisted laser desorption / ionization time of flight (MALDI-TOF) mass spectrometry (MS). GSH, a well-known major antioxidant and reducing agent in living body, exists in high concentration in cytosols. Previous studies have shown that curcumin, which is an also well-known antioxidant, affects the GSH level; however, the correlation between their levels has not been well elucidated yet. In our strategy, GSH in cell lysates was captured on maleimide groups of AuNPs and subsequently analyzed by MALDI-TOF MS in the presence of isotopomer GSH (GSH*)-conjugated AuNPs as an internal standard. Then, the comparison of the relative intensities between GSH and GSH* allowed the quantitation of GSH in cells. In this way, GSH levels in mammalian cells were investigated after incubation with curcumin at various concentrations. We believe our strategy can be commonly used for determining GSH levels of cells that are treated differently with exogenous stimulants such as reactive oxygen species, biofunctional natural products, and drug candidates.

Poster Presentation : **ANAL.P-383**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Substrate Binding Studies of Human Cytosolic Adenylate Kinase1 by NMR

GilHoon Kim, Hoshik Won*

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Arginine residues are known to play important roles in substrate binding through the electro-static interaction of positive charge on the Arg side chain with the negative charge of phosphoryl group in many of nucleotide binding proteins. Human cytosolic adenylate kinase1 (hAK1) has some Arg residues necessary for binding its substrates including MgATP and AMP. To investigate the interactions between Arg side chains and the substrate in aqueous solution, we observed the signals of Arg ϵ -NHs of ^{15}N -labeled AK using ^1H , ^{15}N two dimensional NMR. The experiments with HSQC pulse sequence detected 13 signals corresponding to all Arg residues on hAK1. The 6 residue signals (Arg[44], [97], [128], [132], [138] and [149]) playing important roles in substrate binding associated with LID and AMP binding domain out of all corresponding 13 Arg residues were selectively assigned through Arg to Ala substitution. In kinetic studies, the resulting large increases in the $K_{m,app}$ values for AMP^{2-} of the mutant enzymes, the relatively small increases in the $K_{m,app}$ values for MgATP^{2-} , and the fact that the R132A, R138A, and R149A mutant enzymes proved to be very poor catalysts are consistent with the idea that the assigned substrate binding sites. Two substrates, MgATP and AMP, were titrated into wild type hAK1 and mutants to observe the effects on these assigned signals. The addition of AMP affected 4 Arg signals, whose chemical shift took place a down field in the direction on proton dimension whereas the addition of MgATP did few effects. We were able to find that the Arg[44] specifically interact with the phosphoryl group of AMP. The additions of both the substrates augmented significantly the intensity of Arg[149] signal, which had very low intensity on the spectrum of free wild type AK1. Three ϵ -NH signals derived from Arg[123], [132], and [138] were broadened and disappeared upon the Mg-ATP addition. These arginine residues locate on α -helix and the following loop along the moiety of triphosphate of MgATP.

Poster Presentation : **ANAL.P-384**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

High Sensitive Detection of Capsinoids by Capillary Electrophoresis with Laser-induced Fluorescence Detector

Yucheng Sun, Seong Ho Kang^{1,*}

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¹Department of Applied Chemistry, Kyung Hee University, Korea

The performance of capillary electrophoresis (CE) coupled with laser induced-fluorescence (LIF) detector was evaluated for detection of capsinoids in various foods. Commercial capsaicin and dihydrocapsaicin were used for the evaluation of buffer concentration, pH value, applied voltage, and limit of detection (LOD). Under the optimal condition using 20 mM 2-(cyclohexylamino)ethanesulfonic acid (CHES)-2.2 mM sodium dodecyl sulfate running buffer (pH 10) with injection time of 10 s, the LOD was evaluated to 1 pM for capsaicin and 3 pM for dihydrocapsaicin in short analysis time and high resolution. In addition, CE equipped with UV-vis absorption was presented for comparing the LOD resulting 5 nM for capsaicin and 8 nM for dihydrocapsaicin which showed poorer sensitivity than LIF. Finally, the accessible CE-LIF system was exploited for analyzing real sample of kimchi and chili pepper, the result with short migration time and no loss of resolving power exhibited high agreement to standard capsinoids which were completely distinguished from various similar structured components. The developed rapid and high sensitive CE-LIF method should provide user-friendly on-line detection of capsinoids in various foods.

Poster Presentation : **ANAL.P-385**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A new mixed-mode stationary phase based on silica monolith particles for the separation of peptides in HPLC

Genlin Sun, Won jo Cheong*

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Partially sub-1 μ m silica monolith particles have been prepared by sol-gel reaction followed by differential sedimentation. A mixed mode stationary phase was prepared by chemical derivatization of the particles with a layer of copolymer composed of N-phenyl acrylamide and polystyrene. First, the particles were reacted with 3-chloropropyl trimethoxysilane followed by sodium diethyldithiocarbamate (SDDC) to introduce an initiator moiety. Then, the copolymer layer was immobilized on the initiator attached silica monolith particles via reversible addition-fragmentation transfer (RAFT) polymerization. The resultant phase was packed in glass lined stainless steel micro-columns (1.0 mm x 150 mm) and evaluated for the separation of a mixture composed of five peptides (Trp-Gly, Thr-Tyr-Ser, angiotensin I, isotocin and bradykinin). The effect of ligand mixing ratio (N-phenyl acrylamide vs styrene) on the chromatographic performance of mixed-mode stationary phase was examined. The number of theoretical plates (N) as high as 33,600 plates/ column was achieved for the five peptides using the optimized mixing ratio. Three columns were packed with three different batches of stationary phase to check the column to column reproducibility and the reproducibility in separation efficiency was at least better than 3.0%.

Poster Presentation : **ANAL.P-386**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Multi-channel Microchip Electrophoresis for Rapid Screening of Glutathione S-transferase Polymorphism Genotyping

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¹Department of Applied Chemistry, Kyung Hee University, Korea

A voltage programming (VP)-based microchip electrophoresis (ME) method was developed to detect specific sizes of DNA fragments. The optimum condition was deliberated on a single-channel microchip and was then applied to a multi-channel microchip for simultaneous high-throughput detection. Glutathione S-transferase (GST) polymorphism genes (M1/M1 = 215 bp/215 bp, M1/T1 = 215 bp/480 bp, and T1/T1 = 480 bp/480 bp) extracted from human blood were amplified by polymerase chain reaction and were introduced into the multi-channel microchip. Target DNA molecules amplified by only 10 PCR cycles could be detected by the VP-based multi-channel ME, but not by slab gel electrophoresis. Besides, the migration time for ME was less than 15 s which was 700 times faster than SGE. Furthermore, internal control (312 bp) was added for further identification of target DNA. The presented modality was demonstrated to be effective and rapid for highly sensitive and high-throughput screening of GST genes.

Poster Presentation : **ANAL.P-387**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development and Application of a syringe pump based r-FIA technique: Determination of Phosphate in Water

Sandag Batbileg, Ra-Yun Kim, In-Yong Eom*

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There are many nutrients such as phosphate, nitrate, ferrous ions and their existence are closely related to biochemical reaction of planktones. Phosphate is one of the important nutrient which is the 11th richest element in Earth. Phosphate is also one of the major sources to cause eutrophication from the surface of rivers or lakes. Due to those reasons, it is very important to develop a monitoring system to those nutrients' concentrations in a longterm periods. Conventionally, segmented continuous flow analyzer, ion chromatography, atomic absorption spectroscopy, and AA-MS have been widely used for this purpose. But these instruments are bulky, complex, and professional operation needs so they are more useful in laboratory environment. Development of simple, small, and robust analyzer is always favorable to monitor one or even multi analytes including nutrients, anions, and metal ions. For this purpose, the reverse flow injection analysis (r-FIA) technique is well suited. This technique has an advantage for long term monitoring of analytes in water system which is always sufficient for analysis. At the same time, it can lower the analysis cost by saving the amount of reagent. Usually, r-FIA has better sensitivity compared to the conventional FIA technique. Here, we report r-FIA which used a precise syringe pump to prepare reagent as well as to inject it to the flow system. Home-made heater system was used to reduce the reaction time. IR LED (nominal wavelength 880 nm) was used as solid state light source. Linearity was 30 ppb to 1 ppm with a r-squared value of 0.99. LOD was 10 ppb but this is expected to be lowered by enhancing reaction kinetics. This system is also used to determine metal (i.e. copper and zinc) ions with a small modification of the r-FIA system.

Poster Presentation : **ANAL.P-388**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Preparation of borovanadate system as cathode material for lithium ion batteries

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Lithium-ion batteries are the most important energy storage system for wide applications in electronic portable devices and hybrid electric vehicles. Lithium ion battery consists of four major components such as anode, cathode, electrolyte, and the separator. During the charging process, lithium ions are released from the cathode and transferred to anode through the electrolyte, and this process is reverse during the discharge process. As a cathode material of Li-ion battery, typical vanadium-containing phosphate, $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (LVP), has a high theoretical specific capacity of 197 mAh g^{-1} for the multiple valence state of the vanadium element. In addition, vanadium-contained phosphate has excellent thermal stability and contributing to good cycle stability during the charge and discharge processes. In this study, a lithium borovanadate system, which is a vanadium-contained borate, was prepared via sol-gel method. And its electrochemical properties of samples were investigated. The electrochemical properties of samples were investigated through lithium extraction/inserting processes using galvanostatic charge/discharge and cyclic voltammetry (CV) measurements so as to investigate for Li^+ ion transfer between the active electrode materials.

Poster Presentation : **ANAL.P-389**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Low-cost plastic devices for drug-resistant pathogen detection in point-of-care setting

Jihyo Park, Seonki Hong*

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World health organization (WHO) warns against ‘post-antibiotic’ era as a consequence of the rapid emergence of drug-resistant pathogens, so called superbugs, that are not treated by most of antibiotics. Advanced diagnostic techniques allow clinicians to prevent inappropriate prescribing and overuse of antibiotics which may delay the emergence of life-threatening pathogens. In this study, we aim to develop a low-cost plastic device for rapid and accurate pathogen detection. We applied a nature-inspired material-independent biosilicification process on the surface of plastics that is difficult to be functionalized by conventional surface chemistry due to intrinsic hydrophobicity and lack of functional groups for bioconjugation. By this approach, the surface of polycarbonate and polypropylene-based plastic devices with micro-pillar structure were successfully decorated by silica so that we could selectively enrich bacterial RNA from whole lysate on the surface of devices. Surface-enriched RNA was further detected by on-chip colorimetric loop-mediated isothermal amplification (LAMP) within 30 minutes.

Poster Presentation : **ANAL.P-390**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Preparation of lithium vanadium borate by solid-state method as a cathode for lithium-ion battery

Khoirul Umam, Youngil Lee*

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The solid-state reaction method has been conducted to prepare of lithium vanadium borate (LVB) as a cathode for lithium-ion battery. Carbon coated LVB has been successfully synthesized to improve the conductivity. Various temperatures are given during the sintering process to reach the highest performance. Prepared LVB has been characterized by X-ray diffraction and ^7Li magic angle spinning NMR spectroscopy. Cyclic voltammetry and long cycle performance have been investigated by charge and discharge instrument with various of C rates.

Poster Presentation : **ANAL.P-391**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of vanadium based polyanion cathode materials for lithium-ion battery

Minsoo Ji, Youngil Lee*

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Lithium-ion batteries are promising energy storage technologies for portable electronic devices such as smart phones, camcorders, and laptops. Lithium vanadium pentoxide has been extensively studied as cathode material in lithium-ion batteries due to its ability for accept lithium ions. However, there is a disadvantage that structural instability occurs when a lot of lithium ions accepted. For this reason, we have replaced borate anion and synthesized carbon-coated lithium vanadium borate which may be expected enhancement of electrochemical properties and structural stability. We expected that the borate anion would lead to increase in structural stability and electric conductivity. The electrochemical properties of lithium vanadium borate were characterized by cyclic voltammetry (CV) measurement for reversibility of lithium extraction/inserting processes.

Poster Presentation : **ANAL.P-392**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Ratiometric Measurement of Intravesicular pH Detection Using Fluorescent dye

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Intravesicular pH detection was done by using Hybrid Proteoliposome that change inside of the vesicle's pH through Proteorhodopsin. If we use light to the Hybrid Proteoliposome, intravesicular pH changes. To detect intravesicular pH changes, We did ratiometric measurement method using Carboxy-SNARF-1 fluorescent dye. SNARF-1 has one excitation wavelength(488nm) and dual emission wavelength at different forms (protonated and unprotonated). After calibrate fluorescent emission intensity for each pH 6~9.5, and make ratio graph of dual emission wavelength intensity. After that, we measured artificial cell's fluorescent intensity by confocal microscope using one laser and several different wavelength range(acidic form at 560-600nm, basic form at 620-660nm). So We can know the approximate concentration of two kind of SNARF-1 forms. And using fluorescence intensity values to 'Two-Wavelength-Ratio Equation'(below), we can detect intravesicular pH. $[H^+] = K_a (R-RA^-) IA^- (\lambda_2) / (RAH-R) IA_H \lambda_2$. $R = I_{\lambda_1} / I_{\lambda_2}$. $RAH = IA_H \lambda_1 / IA_H \lambda_2$ (the limiting value of R for acidic form). $RA^- = IA^- \lambda_1 / IA^- \lambda_2$ (the limiting value of R for basic form).

Poster Presentation : **ANAL.P-393**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhanced SAMDI Efficiency for the analysis of biomolecule-conjugated alkanethiolates by using tetrahydrofuran

Hyunook Kang, Woon-Seok Yeo*

Department of Biotechnology, Konkuk University, Korea

In this poster, we demonstrated the improvement of efficiency for the analysis of self-assembled monolayers (SAMs) of alkanethiolates on gold with matrix-assisted laser desorption/ionization time-of-flight mass spectrometry, termed SAMDI-TOF MS. Previously, we found that tetrahydrofuran (THF) highly compromised the monolayer stability, and thus, induced unusually fast exchange of alkanethiolates of SAMs with other alkanethiols in the solution. As such, the use of THF for preparing matrix solution facilitated the desorption of alkanethiolates from the gold and co-crystallization with matrix molecules, and therefore, improved the SAMDI efficiency. We investigated SAMDI efficiency for the analysis of carboxylic acid-, maleimide-, and peptide-presenting SAMs using the various organic matrix solutions in acetonitrile, ethanol, methanol, and THF. In addition, biomacromolecule-conjugated SAMs such as GST, alpha-casein, and beta-casein were also analyzed. We found that SAMDI efficiency was highly improved when THF was used as a matrix-dissolving solvent as expected. Since SAMDI technique is fast, simple, and amenable to wide range of (bio)molecules on SAMs on gold, we believe our study would be highly informative and practical in various applications using SAMs on gold platforms.

Poster Presentation : **ANAL.P-394**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Evaluation of Fuzzy Rule Building Expert System Tree and Restricted Boltzmann Machine for NIR Spectroscopic Identification of Geographical Origins of Agricultural Products

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²*Department of Chemistry, Hanyang University, Korea*

Fuzzy rule building expert system tree (FuRES) and Restricted Boltzmann machine (RBM) have been evaluated as a potential method for NIR spectroscopic identification of geographical origins of agricultural samples. FuRES is a tree algorithm with fuzzy expression of classification entropy. FuRES has benefits from simulated annealing and gradient optimization. Restricted Boltzmann machine (RBM) is a restricted form of Boltzmann machines with gradient descent and back-propagation. It can be trained in either supervised or unsupervised ways, depending on the task. In this study, RBM is applied for supervised classification and unsupervised way to extract features. For the evaluation, NIR spectra of imported and domestic agricultural samples (8 different samples: adzuki, angelica root, bellflower root, bracken, carrot, green kernel black bean, kidney bean and perilla seed) were used. For each sample, the discrimination accuracies were acquired using both methods and compared with those using conventional methods such as linear discriminant analysis (LDA) and support vector machine (SVM). The advantages and disadvantages of FuRES and RBM, and their potential in vibrational spectroscopic discriminant analysis will be discussed.

Poster Presentation : **ANAL.P-395**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of integrated Correlative Light and Electron Microscope

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Light microscopes can obtain color information but do not provide resolution below submicron. The electron microscope can provide much higher resolution information in nanometer scale, but it has the disadvantage that the image is grayscale. As a result of changing the source of the microscope from light to electrons, high resolution was achieved, but the most important visual information, the color, was lost. In order to solve these problems, recently a Correlative Light and Electron Microscope (CLEM) has been developed by integrating an light microscope and an electron microscope, and related researches have been actively conducted. Capability of acquiring color-based information as well as nanometer scale surface information of a sample gives users a new possibility in their research. Previously, samples were observed by a light microscope, and then transferred to an electron microscope. However, in this case, the time and space efficiency is poor, and the sample can be damaged during the transfer of the sample. However, the microscope developed by ourself has the advantage of reducing the chance of sample damage and observation time because there is no need to move the sample by operating the light microscope and electron microscope simultaneously inside the vacuum. For the identification of defects such as quantum dots and LEDs, a resolution of less than a micrometer(μm) is required, but an light microscope can not show microscopic defects due to the resolution limit. Since the light and the electron beam provide complementary information, it is required to develop a fusion microscope that observes the sample with visible light and enlarges the suspected region using electrons. In this study, we introduce an iCLEM that can present images in real time by integrating light microscope and electron microscope into one system. The light path of the light microscope is positioned inside the optics of the electron microscope so that the coaxial alignment is achieved. This makes it possible to acquire images of fluorescent images and electron microscopes at high magnifications without moving the sample in the vacuum chamber. The iCLEM may provide researchers with diverse applications in inspection and analysis where a wider resolution spectrum is required in the future.

Poster Presentation : **ANAL.P-396**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Mini-columns of 5 cm length packed with very fine C18 silica monolith particles.

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Very fine silica monolith particles were prepared by sol-gel reaction, drying, smooth grinding, and calcination followed by a series of differential sedimentation. The size of the selected particles was less than 2.5 μm . The particles were classified into 3 groups: the group of sub-1 μm particles, the group of average ca 1.5 μm particles, and the group of average ca 2 μm particles. The particles of each group were chemically modified with C18 ligand and end-capped. The resultant phase was packed in glass lined stainless steel narrow bore columns (1.8 mm x 50 mm). The chromatographic performance and their potential application in fast analysis have been comparatively studied.

Poster Presentation : **ANAL.P-397**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

The study of Thermal Property of RDX according to particle size by ARC and DSC

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Accelerating rate calorimeter(ARC) and differential scanning calorimeter(DSC) are important methods for studying the thermal behavior of energetic materials. In comparison to DSC, which uses mostly a forced linear heating up of the sample, ARC determines the self heating of the sample in a pseudo adiabatic environment. Techniques of thermal analysis such as ARC and DSC have been used in the study of activation energy(E_a) and frequency factor(A) depending on the particle size of RDX. Activation energy (E_a) and frequency factor (A) depending on the particle size of RDX were studied by ARC and DSC. Activation energy(E_a) and frequency factor(A) of DSC were calculated by Kissinger's method and Vyazovkin method with heating rate from 2 to 8°C/min. Studies of the thermal behavior of RDX by ARC and DSC indicated that the Cl-3(large crystal) has better thermal stability than Cl-5(small crystal).

Poster Presentation : **ANAL.P-398**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Quantitation of DNA Using Integrated Nanogap Biosensor.

Ri Yu, Cho Yeon Lee¹, Wan Soo Yun^{1,*}

Sungkyunkwan University, Korea

¹Department of Chemistry, Sungkyunkwan University, Korea

Nanogap sensors have the advantage of sensitive detection using electrical signals, but difficult to quantify due to irregular changes in conductance. Recently, however, we were paper has been published a digital domain analysis method that can quantify target molecules through integrated nanogap devices and on-device-percentage (ODP). In this study, we quantified DNA by applying integrated nanogap sensors and improve the detection speed of existing sensors. We were applying the previously described integrated nanogap device for quantitatively sensing and then nanogap electrodes integrated on the device are distinguished by “On” and “Off” according to the change of conductance, and then ODP values were measured according to the concentration. As a result, nanogap sensor with ODP system was demonstrated the rapid detection and quantification of low-concentration DNA, which was not seen in previous nanogap sensors.

Poster Presentation : **ANAL.P-399**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Determining the 3D orientation of individual anisotropic nanoparticles in live single cell by correlative light Sheet super-resolution microscopy

Suresh Kumar Chakkarapani, Seong Ho Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Gold nanorods (AuNRs), are actively employed as an imaging probes because of their special nonblinking and nonbleaching absorption, scattering, and emitting properties that arise from the excitation of surface plasmons. Herein, we report a novel light sheet microscopy that detects three-dimensional orientation at the nanoscale via polarization encryption of individual AuNRs. By simultaneously imaging the turn off-on signals as a function polarization, 3D super-resolution imaging was achieved intracellular. The spatial orientation of many individual AuNRs was detected in situ and in real-time, enabling its use as a technique for high-throughput imaging. Furthermore, 3D images of individual nanoparticles were resolved in intracellular aggregated regions, resulting in as low as 64 nm axial resolution and 28 nm spatial resolution. These unique features make the orientation probes proposed, as an outstanding candidate for super-resolution optical imaging in materials science and biological applications.

Poster Presentation : **ANAL.P-400**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Plasmon confined optical field enhanced native fluorescence for concurrent single-molecule detection of capsaicinoid analogues

Suresh Kumar Chakkarapani, Seong Ho Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

A high-sensitivity single molecule detection with surface plasmon field-enhanced fluorescence spectroscopy (SPFS) was employed to detect native fluorescence from capsaicinoids. The relative fluorescence intensity of the capsaicinoids were too low for single molecule detection, therefore its fluorescence was enhanced by the spectral overlap of suitable plasmon nanoparticle. By using the SPFS method, the detection limit for capsaicin was 30 zM, dihydrocapsaicin was 90 zM, and the dynamic range was estimated to be at least five digits. Considering the capsaicin and dihydrocapsaicin as the major capsaicinoid analogues, both were simultaneously detected at single molecule level by a ratio-metric quantification. These results suggested that high-sensitivity ratio-metric SPFS single molecule sensor systems might become a powerful tool for the native fluorescence detection.

Poster Presentation : **ANAL.P-401**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Sensing of mercury ions with gold nanoparticles using depolarized light scattering

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Sensing of mercury ion(Hg^{2+}), a well-known toxic pollutant, has been investigated with various techniques due to its danger to the environment. Among them, the resonance light scattering (RLS) using gold nanoparticles (AuNPs) has shown high sensitivity to the concentration of mercury ion because the aggregation of AuNPs induced by the mercury ion can greatly enhance the RLS intensity. However, its application to real samples should be carefully designed because of the possible significant background light scattering from large dielectric particles which can exist in the target sample solution. In contrast to RLS, the depolarized light scattering (dPLS) can be dominantly generated from the plasmonic AuNPs, not from dielectric particles. Therefore, dPLS can effectively minimize the contribution of dielectric particles in the solution to the measured scattering signal in principle. In this presentation, the sensitivity of RLS and dPLS techniques for the concentration of mercury ion are quantitatively compared using the citrate-stabilized AuNPs as probes. This study can be helpful for the design of efficient optical technique using plasmonic nanoparticles for their sensing applications. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (NRF-2015R1D1A1A01058604)

Poster Presentation : **ANAL.P-402**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Optimization of phosphoproteome analysis for low sample amounts using HAMMOC based TiO₂ microcolumn coupled to online 2D-NCFC-RP/RPLC system

Suhwan Kim, Sang-Won Lee^{1,*}, Hangeore Lee¹, Jeonghei Choi¹

Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

Phosphorylation of proteins is one of the most prominent posttranslational modifications (PTMs) and plays essential roles in biological processes. However, as the stoichiometry of protein phosphorylation is generally low, minimizing suppression effects from highly abundant unmodified peptides is essential. The optimal phosphoproteome analysis requires two major improvements: efficient and un-biased phosphopeptide enrichment method with high specificity and highly efficient and sensitive phosphopeptide separation with minimal loss. In this study, we employed an aliphatic hydroxy acid modified metal oxide chromatography (HAMMOC) using a TiO₂ microcolumn for efficient and specific phosphopeptide enrichment. This method showed high enrichment selectivity because aliphatic hydroxy acids, such as lactic acid, is weak enough to allow phosphate groups to preferably bind to metal oxides, yet at the same time is strong enough to prevent carboxylic groups of acidic non-phosphorylated peptides from binding to the beads. Also, under acidic conditions, titanium dioxides show hydrophilic interaction chromatography (HILIC) properties and anion exchange properties, allowing the HILIC and ERLIC elution for both mono- and multi-phosphorylated peptides. The enrichment phosphopeptide samples were sensitively analyzed by using a fully automated dual online 2D-NCFC-RP/RPLC system that bypassed labor-intensive manual sample processes and resulted in peptide fractions of similar complexity being subsequently analyzed by RPLC experiments. Due to the all online feature of the fully automated dual online 2D-NCFC-RP/RPLC system, the optimized method was demonstrated to result in high coverage of phosphorylation sites from a limited amount of proteome sample.

Poster Presentation : **ANAL.P-403**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical Dopamine Sensor Using Nano/Micro Gap Interdigitated Electrodes

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Department of Chemistry, Sungkyunkwan University, Korea

Highly sensitive detection of dopamine is important because dopamine is an essential neurotransmitter and a clinically valuable diagnostic indicator. The electrochemical sensor is one of the powerful methods for the detection of dopamine due to their redox activity. The application of interdigitated electrodes (IDEs) enables the amplification of electrochemical signals which results in lower detection limits in the biosensor. In this study, we designed the dopamine sensor with IDEs has various gap sizes from 10 μm to 500 nm. We can analyze the correlation between gap size and electrochemical signal and detect dopamine at nanomolar concentration level.

Poster Presentation : **ANAL.P-404**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Physicochemical characterization of glutamate decarboxylases from *Lactobacillus brevis* (*L. brevis*)

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Peñarrieta³, Lars Nilsson^{1,*}, Seungho Lee^{4,*}**

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Lactobacillus brevis (*L. brevis*) strains are present both in fermented food as well as in the human gut. These strains are considered food grade bacterium and confer positive effects to the human health. They are particularly interesting due their capability to produce gamma aminobutyric acid (GABA), a bioactive compound mostly known by its inhibitory role in the neurotransmission mechanism. However, recent, both *in vivo* and *in vitro*, evidences support a number of new potential biological functions of GABA, including anti hypertension, anti-diabetes and others. The glutamate decarboxylase (GAD) is an enzyme responsible for synthesis of GABA from glutamic acid. Interestingly, the genome of some strains of *L. brevis* encodes two different GADs: GadA and GadB. The physicochemical characterization of these enzymes will contribute to understand the molecular basis of the GABA production and therefore will set the basis for further applications of glutamate decarboxylases in the biotechnological production of functional ingredients for food and feed. The highest activity of GADs was observed when the enzyme forms hexameric oligomerers. Thus, the study of the physicochemical factors that affect stability of the oligomers, such as pH, temperature, type of salts and ionic strength are fundamental to establish the suitable conditions for the optimal enzymatic activity. Recently we have developed analytical methods based on asymmetrical flow field-flow fractionation (AsFFFF) and light scattering techniques that allows the study of both oligomerization as well as aggregation of GadB (Choi, et al. 2018). Currently we are characterizing GadA and also the effect of the factors mentioned above in the enzyme kinetics.

Poster Presentation : **ANAL.P-405**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Analysis of anthocyanin in red wine by asymmetrical flow field-flow fractionation (AsFIFFF) and HPLC

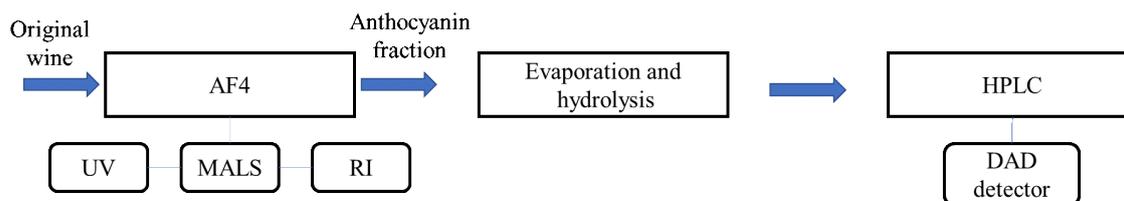
Dongsup Song, E. Osorio-Macias Daniel¹, Jaeyeong Choi¹, J. Mauricio Peñarrieta², Lars Nilsson¹, Seungho Lee*

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Abstract : Anthocyanin is an antioxidant, and is of various types. In this study, the type and the content of anthocyanin in red wine were determined. For comparisons, five commercial red wines were chosen, one French wine and four Argentinian wines. First, a wine sample was injected into an asymmetrical flow field-flow fractionation (AsFIFFF) to separate the components in the sample. Then the anthocyanin fraction from AsFIFFF fractogram was collected, and injected into HPLC (C18, 2.7 $\mu\text{m}\times 100$ mm) for quantitative analysis after a sample preparation procedure shown in Scheme 1 below, which includes evaporation and hydrolysis^[1]. Significant differences were found among the tested wine samples of various sources in both the type and the content of anthocyanin. AsFIFFF provided an useful tool for separation of anthocyanin from red wine, and thus for HPLC analysis of anthocyanin, while the size-exclusion chromatography (SEC) suffer from interactions between the wine components and the stationary phase. **References** : [1] A. Vernhet, S. Dubascoux, B. Cabane, H. Fulcrand, E. Dubreucq and C. Poncet-Legrand, *Anal Bioanal Chem* 2011, 401, 1559–1569.



Scheme 1. experimental procedure

Poster Presentation : **ANAL.P-406**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of facile mercury detection via fluorescein-based dye

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Mercury, which exists in the environment as inorganic and organic mercurial species, is known to be highly toxic in most forms and can cause DNA damage, mitosis impairment, and permanent damage to the central nervous system. Because of modern industrial activities, mercury and mercury species are continuously released into the environment from a variety of sources such as coal-fired power plants and gold mines. Therefore, it is important to detect mercury sensitively and selectively. Recently, the optical determination or visualization of important chemical and biological species has attracted much research interest. Because of the high toxicity of mercury and mercury species to humans, many Hg²⁺-selective signaling or visualization probes have been developed. Fluorescein and its related derivatives have been widely employed as signaling handles for molecular imaging and chemosensing applications. In this research, mercury-selective signaling probe based on 2,7-dichlorofluorescein (DCF) has been reported. This probe is easily synthesized by one-step reaction of 2,7-DCF with Phenyl chlorothionoformate under room temperature condition. The signaling of this probe is due to Hg²⁺-induced hydrolysis of thionocarbonate moiety to produce 2,7-DCF. This hydrolysis restores the property of 2,7-DCF. In 50% DMSO aqueous solution, this probe showed absorbance signal at specific wavelength significant turn-on type fluorescence signal toward Hg²⁺ only. In addition this probe was hardly affected by other coexisting cations or coexisting anions. Finally, this probe also showed fluorescence signal in cell.

Poster Presentation : **ANAL.P-407**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

A Proteomics Study to Investigate Oncogenic Roles of PAF in Lung Adenocarcinoma

Jiwon Hong, Moon Jong Kim¹, Do-Woon Nam, Jingi Bae, Dong-gi Mun, Seunghoon Back, Su-Jin Kim, Hokeun Kim, Jae-II Park^{1,*}, Sang-Won Lee^{*}

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Lung adenocarcinoma (LUAD), contributing to 40% of all cancer types, is known as the most common category in lung cancer. Proliferating cell nuclear antigen-associated factor (PAF) is specifically expressed in tissue stem cells and cancer cells including LUAD. PAF is associated with cell hyperproliferation, cell plasticity, cell stemness, and gene transactivation in tissue stem cells and cancer. Nonetheless, the pathologic roles of PAF in LUAD remain elusive. In this study, we aim to uncover the oncogenic roles of PAF in LUAD by comprehensive proteomic analyses on both protein and phosphorylation changes in PAF knockdown lung cancer cell lines. Both global proteome and phosphoproteome quantitative profiling were performed on the TMT 6-plex labeled peptide sample from six cell lines (i.e. three control cancer cell lines and three PAF knockdown cancer cell lines). Our deep quantitative profiling experiments resulted in identification of 270,503 distinct peptides of 11,336 protein groups and 21,080 distinct phosphopeptides of 17,461 phosphorylation sites. We are currently identifying proteins and phosphorylations affected by PAF knockdown and their associated cellular pathways, which in turn should lead to better understanding on the tumorigenic roles of PAF in LUAD progression.

Poster Presentation : **ANAL.P-408**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

“Hidden” isocratic elution on a dual online reverse-phase liquid chromatography to increase the utilization of LC-MS/MS experiment time for highly efficient proteomic analysis

Do-Woon Nam, Jeonghei Choi¹, Hangeore Lee¹, Sang-Won Lee^{1,*}

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Reverse-phase liquid chromatography (RPLC) is a method of choice in current proteomics and generally employs a hydrophobic gradient of a mobile phase to efficiently elute peptides. However, in this method, the hydrophilic peptides with little retention to the hydrophobic stationary phase tend to elute at the same time at early gradient, suffering from ion suppression due to the co-eluting peptides. Isocratic elution offers an advantage of separating the low retaining hydrophilic peptides while it is generally not suitable for eluting hydrophobic peptides. In this work, we developed a new separation scheme in which an isocratic elution prior to gradient elution was used and the isocratic elution is “hidden” in the LC-MS/MS experiments time so that the entire experiment time remains the same as if there is only gradient elution being employed. This “hidden” isocratic elution was accomplished by performing the back-flushing sample injection and isocratic elution on one column while RP gradient separation is being executed on the other column on a dual online reverse-phase liquid chromatography (DO-RPLC) system. The duration of the isocratic elution was determined so that the first peptide peak eluting from the column was to be measured by a mass spectrometer, effectively removing lead time in LC-MS/MS measurement. The “hidden” isocratic elution prior to gradient elution on a DO-RPLC system was demonstrated to provide maximum utilization of LC-MS/MS experiment times while accomplishing increased identification of hydrophilic peptides.

Poster Presentation : **ANAL.P-409**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Dispersive Liquid-Liquid Microextraction based on Deep Eutectic Solvent for the HPLC-UV Determination of Resveratrol, Oxyresveratrol and Piceatannol from Wine

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Polyphenols are phytochemicals that exist in various plants and are beneficial to human health. These ingredients prevent aging, protect the skin from ultraviolet rays, improve brain health and prevent dementia. Resveratrol, oxyresveratrol and piceatannol in grapes are typical polyphenols, and grape wine also contains these ingredients. In this study, resveratrol, oxyresveratrol and piceatannol in wine were extracted by deep eutectic solvent based dispersive liquid-liquid microextraction (DLLME) and a method for quantification these polyphenols using high performance liquid chromatography - UV/vis spectroscopy was established. Parameters for sample clean up and concentration were optimized and verified. Experiments were carried out to obtain optimal parameters such as the types and volumes of extraction solvent and dispersive solvent, molar ratio of hydrogen bonding donor and hydrogen bonding acceptor, ratio of deep eutectic solvent and water, the pH effect, and the effect of salt. Chromatographic separation with HPLC/UV-vis was performed using the eclipse XDB-C18 (2.1 mm id × 150 mm length, 4.6 μm particle size) column and gradient elution mode using water and acetonitrile. The established method would be applied to wines sold in the market and monitored.

Poster Presentation : **ANAL.P-410**

Analytical Chemistry

Grand Ballroom, FRI 11:00~12:30

Verification of Biomarker Candidates for High-Risk Diabetes Mellitus

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Center for Proteogenome Reserch, Department of Chemistry, Korea University, Korea

Diabetes mellitus (DM) is a common chronic disease that can cause various complications. Recently, there has been sharply increased in diabetes patients in Korea because of lifestyle change. When high-risk groups are diagnosed in early stage, immediate and suitable treatments can prevent the DM. However, accurate diagnosis in early stage of DM remains difficult due to its symptomless characteristic. Especially, Korean (Asian) have different risk factor for DM from European so that Korean specialized method is needed. We performed experiment using DM high-risk patient samples which were tracked past 10 years for discover DM early diagnosis biomarker specialized to Korean. Our research aims to identify the biomarkers that can predict whether high-risk patients would maintain their condition or develop to DM. Using Q-Exactive mass Spectrometer, parallel reaction monitoring (PRM) was performed on the 80 patient digested serum samples to quantify 84 biomarker candidate proteins which are based on global profiling result. For sensitive and accurate quantification, 100 cm length long column and 200 min LC gradient were used in experiment. Stable isotope labeled peptides (, or AQUA peptides) were used to validate the targets identified in global profiling results and verify the expression changes of the targets.

Poster Presentation : **LIFE.P-411**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Homoharringtonine induces apoptosis in human colorectal carcinoma HCT116 cells via downregulation of Wnt/ β -catenin signaling cascade

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The Wnt/ β -catenin pathway plays an important role in cancer development. Since β -catenin is one of main factors for the survival of colon cancers through maintaining the efficient activation of Wnt-responsive genes such as c-Myc and cyclin D1, the targeting of β -catenin could be a promising approach for treating colon cancers. Therefore, we screened 9,939 compounds and identified homoharringtonine (HHT) as the most potentially active compound to inhibit β -catenin activity. HHT reduced the protein levels of c-Myc and cyclin D1, demonstrating its potential to inhibit β -catenin activity. Time-dependent experiments also suggested that its potential to inhibit β -catenin activity could lead to the caspase-dependent apoptotic death of human colorectal carcinoma HCT116 cells. Inhibitory activity of HHT on the growth of HCT116 cells was also confirmed in colony formation experiment. Notably, among the signaling factors in Wnt signaling and secretion, HHT reduced the expression levels of p-LRP6, LRP, β -catenin, TCF4 and porcupine, but not Dvl, demonstrating that HHT exhibits anti-colon cancer action via inhibiting β -catenin activity. Considering that HHT is being clinically used for treating patients with chronic myeloid leukemia, these results warrant its development as a potential anti-cancer drug targeting colon cancers.

Poster Presentation : **LIFE.P-412**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

A Near-Infrared Fluorescent Probe for Amyloid- β Aggregates

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Jinheung Kim^{2,*}**

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The deposition of amyloid- β (A β) aggregates in the brain is a hallmark of Alzheimer's disease (AD)-affected brain. The toxicity associated with A β aggregation and generated A β aggregates has been gained much attention to elucidate the pathogenesis of AD. To elucidate a relationship between A β species and toxicity, an effective strategy, such as utilization of a fluorescence probe, to noninvasively identify the existence of A β peptides in biological environments is necessary. In this presentation, we will report a new, turn-on near-infrared fluorescent dimethylaminostyrene- and indole-based probe, **1**, for A β aggregates, which consists of a donor- π conjugation-acceptor structure with an A β -interacting moiety. Our probe, **1**, shows a noticeable increase in fluorescence at ca. 710 nm upon treatment of A β aggregates in aqueous media. Moreover, **1** is observed to be nontoxic under imaging conditions and detect A β species in living cells.

Poster Presentation : **LIFE.P-413**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Biochemical Characterization and Structural Studies of engineered novel antimicrobial peptides

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Since the discovery of penicillin, antibiotics have brought benefits such as prolonging human life, treating bacterial infections as well as promoting animal growth, but misuse and abuse of antibiotics have caused serious public health problems and economic losses. In addition, unnecessary prescriptions have caused many side effects, and the most problematic is the emergence of super bacteria with antibiotic resistance. Furthermore, due to the scientific difficulties of development and the rapid emergence of antibiotic-resistant bacteria, new types of antibiotics have not been developed in the past 30 years, and therefore the spread of super bacteria resistant to antibiotics is a matter of time. Thus, antibiotics that work in a completely different way from conventional antibiotics have become necessary, and long-term solutions to these problems include antimicrobial peptides produced by all organisms, from bacteria to vertebrates and invertebrates. We have successfully identified the structure and activity of Lactophorin (LPcin), an antimicrobial peptide found in bovine milk, through expression using recombinant DNA technology, purification using various biophysical techniques, and structural studies using liquid/solid-state NMR. Based on this, we constructed a total of 20 analogs library through conservative sequence modification to develop new antimicrobial peptides with shorter length and improved antimicrobial activity than conventional LPcin. Among them, six new antimicrobial peptides were selected through bacterial killing assays and growth inhibition assays, and each peptide was obtained a high purity, sufficient amount for structural studies by optimization of the expression and purification process. In addition, each peptide identified its potential as a new antibiotic through hemolysis assay and cytotoxicity assay, and to investigate the relationship between active-structure by conducting a 3D topology structure study using liquid/solid-state NMR.

Poster Presentation : **LIFE.P-414**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Nucleotide hydrolysis and nucleic acid unwinding analysis of Middle East Respiratory Syndrome coronavirus helicase

Yong-Joo Jeong

Department of Applied Chemistry, Kookmin University, Korea

An infectious respiratory disease, Middle East Respiratory Syndrome (MERS), is caused by a modified coronavirus. MERS coronavirus is a (+) single stranded RNA virus. Of the several non-structural proteins produced from the virus, NTPase/helicase plays an important role in viral replication. Helicases are molecular motors that separate double-stranded nucleic acids using the energy generated by NTP hydrolysis. In the present study, we analyzed the NTP hydrolysis and nucleic acid unwinding activities of MERS helicase. Based on the results, we developed an efficient high-throughput screening system to find inhibitory molecules.

Poster Presentation : **LIFE.P-415**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Application of the Red Fluorescent Protein as an Indicator of Recombinant Protein Production in Escherichia coli

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Department of Chemistry, Sejong University, Korea

The discovery of green fluorescent protein has brought a new era in cell biology by enabling scientists to monitor various cellular processes in living systems in real time via optical microscopy by fusing the fluorophore moiety to many proteins and enzymes of interest. Researchers have developed a broad spectrum of fluorescent proteins, covering the entire visible light range from blue to green to yellow to red colors. We have employed the red fluorescent protein (mCherry) to provide the visualization of the target gene expression in Escherichia coli. The mCherry gene was tagged right next to the maltose-binding protein (MBP) which was widely used as a fusion partner to provide high yield and solubility. The target gene was inserted behind the His-Tag, and the tagged protein was designed to be cleaved off of the MBP-mCherry inside the cell by the constitutively expressed TVMV protease. The red color became clearly visible after the induction signal was turned on, showing that the expression of the MBP-mCherry-target gene had started and went well. The target protein was successfully purified by the Ni-NTA column. This work has been supported by Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2017R1D1A1A02017545). References 1. Hui, C.-Y., Guo, Y., Zhang, W., & Huang, X.-Q. (2018). Rapid monitoring of the target protein expression with a fluorescent signal based on a dicistronic construct in Escherichia coli. *AMB Express*, 8, 81. <http://doi.org/10.1186/s13568-018-0612-52>. Su, W. W. (2005). Fluorescent proteins as tools to aid protein production. *Microbial Cell Factories*, 4, 12. <http://doi.org/10.1186/1475-2859-4-123>. Using green and red fluorescent proteins to teach protein expression, purification, and crystallization. *Biochem Mol Biol Educ* (2008) 36(1), 43. <http://doi.org/10.1002/bmb.117>

Poster Presentation : **LIFE.P-416**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhancing enantioselectivity of *Candida antarctica* lipase B towards but-3-yn-2-ol

Seonghyeon Yi, Seongsoon Park*

Department of Chemistry, Sungshin University, Korea

Candida antarctica lipase B (CAL-B) is one of the most widely used lipases for preparation of chiral building blocks because CAL-B possesses high enantioselectivity towards many secondary alcohols. However, CAL-B exhibits low enantioselectivity towards secondary alcohols bearing small substituents (i.e. but-3-yn-2-ol ($E = 6$) and 2-butanol ($E = 7$)). In this study, we present improvement of enantioselectivity of CAL-B toward but-3-yn-2-ol and 2-butanol. The medium binding pocket was altered to reduce the space of the medium binding pocket of CAL-B. The mutant enzymes exhibited higher enantioselectivity ($E > 200$ and $E > 20$) towards but-3-yn-2-ol and 2-butanol, respectively, compared to those of the wild type enzyme.

Poster Presentation : **LIFE.P-417**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Identification of a topologically distinct depsipeptide with multiple bicyclic core peptides expands the diversity of the microviridin-like modified peptides

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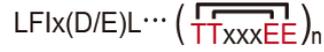
Microviridins represent a ribosomally synthesized and post-translationally modified peptides (RiPPs) family that contains intramolecular ω -ester and/or ω -amide bonds between two side chains of the peptide. Most currently known microviridin-like peptides have one consensus sequence pattern and a unique ring topology. To expand the scope of the microviridin-like peptides, we determined the crosslinking connectivity of a novel modified peptide, mTgnA, and two other homologs. They contain a novel consensus sequence for the core peptide, TxxTxxxExxDxD, and the leader peptide, KPYxxxYxE, of which the core peptide forms a distinct hairpin-like bicyclic structure by the cognate ATP-grasp enzyme. In order to determine the full crosslinks connectivity of the three modified core motifs in mTgnA the ester-specific reactions and tandem mass spectrometry were used. The crosslinking reaction proceeded from the inner to outer rings, and was selective for acidic amino acids identities. We suggest that the scope of microviridin-like RiPPs is beyond the one found in microviridins and to name this expanded family of RiPPs with the microviridin-like modification as the “omega-ester containing peptides (OEPs)”.

OEP(Omega Ester-containing Peptide)

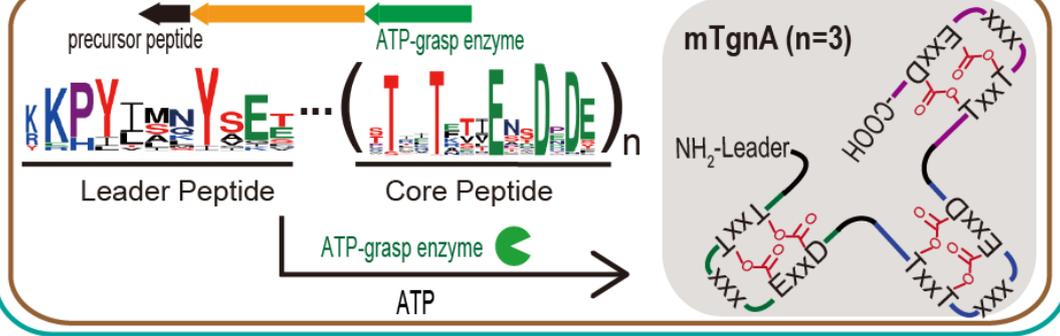
Microviridin group



Plesiocin group



Thuringinin group



Poster Presentation : **LIFE.P-418**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Characterizing Hetero-oligomer of Amyloid-beta and Alpha-synuclein with Bio-AFM

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Alzheimer's Disease (AD) and Parkinson's Disease (PD) are neurodegenerative diseases resulting in progressive degeneration or death of neuron cells. These are associated with the aggregation of peptides, 'amyloid-beta (A β)' and 'alpha-synuclein (α -syn)'. It is believed that A β and α -syn oligomers are intermediates in the fibril formation, and both oligomers and fibrils are primarily responsible for the pathogenesis. Further study showed that rate of the oligomerization (or aggregation) increases when A β and α -syn co-exist, and the co-existence causes the diseases even worse. It is very likely that hetero-oligomers could be formed, but presence and structure of the hetero-oligomers have not been elucidated. Herein, we employed atomic force spectroscopy with a liquid cell to characterize the hetero-oligomers generated in vitro. For comparison, homo-oligomers were prepared separately. In particular, antibodies recognizing N-terminal of A β and N-terminal of α -syn were conjugated at AFM probes, and the specific interaction between the antibodies and surface of the oligomers was followed^{1,2,3}. After adsorbing the oligomers on mica surface, a tip tethering A β antibody was used to get high resolution force maps of a target oligomer, and subsequently another tip tethering α -syn antibody was brought to the same target for the examination. The overlaid map revealed that specific unbinding events with respect to two different antibodies were observed within an oligomer, and it holds for all sizes under investigation. Because homo-oligomers were not observed at all, it can be said that formation of hetero-oligomers is strongly favored. It is intriguing to note that the percentage of recognizing pixels for α -syn increases in comparison with the α -syn homo-oligomer, suggesting a different mode of aggregation for the hetero-oligomerization. We believe that such structural information helps to understand the relationship between the misfolded proteins and the pathogenesis in brain.

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Poster Presentation : **LIFE.P-419**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

3D bioprinting of bifurcating vessels for hierarchical vasculature

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Despite the significant advancements in tissue engineering to mimic native tissue constructs, fabrication of bifurcating vessels and vascularized tissue constructs still pose a great challenge. The importance of vascular networks in tissue constructs is that vascularization provides nutrient with and remove cellular waste from the cells in tissue. Here, we present a novel method to bioprint bifurcating vessels and develop hierarchical vasculature. In particular, we designed a diffusive bioprinting method by incorporating calcium chloride in Pluronic F127 (PFCa) and casting of alginate/gelatin mixture over the extruded PFCa ink. Pluronic F127 as well as blend with calcium chloride shows Bingham plastic properties which enable preservation of extruded filamentary shape and bifurcation of the vessels. After casting alginate/gelatin mixture on extruded PFCa, calcium circumferentially diffuse and crosslink alginate, yielding a tubular hydrogel construct that physically mimics vessels. The structural properties of the vessels are tuned by changing the calcium diffusion time and the concentration of calcium in PFCa. This diffusive bioprinting technique enables bifurcation of the vessels and hierarchical vasculature that obey Murray's law, such that the cost for transport and maintenance of the transport materials is minimized. The bifurcating vessels and hierarchical vasculature could improve the material flow between cells which in turn promote cell viability over time in artificial tissue constructs.

Poster Presentation : **LIFE.P-420**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Quantitative Analysis of DISC1 in a Single Cell with Atomic Force Microscopy

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Schizophrenia is a mental disorder characterized by abnormal social behavior and failure to understand what is real. Several studies have shown that unregulated expression or altered protein structure of disrupted in schizophrenia 1 (DISC1) may predispose individuals to the development of schizophrenia, clinical depression, bipolar disorder, and other psychiatric conditions. Therefore, identification of protein level or post-translational modifications of DISC1 can provide targets for diagnosis and treatment of schizophrenia. Especially, post-translational modifications of DISC1 have been studied as a mechanism to regulate the interaction with these proteins under specific conditions. Recently, several studies have been discovered that phosphorylation of DISC1 plays an important role in the process of neural development. Conventional methods for protein analysis including western blotting, ELISA, and immunofluorescence have some problems that they have low detection limit and use fluorescent molecules. Also, we can't know the information about a single cell because they measure ensemble average of molecules. Therefore, we analyze target proteins which are DISC1 and phospho-DISC1 in a single cell using atomic force microscopy (AFM). AFM have the capability to detect one to one interaction between antigen and antibody. By using nanoarray of fluidic force microscopy (FluidFM), trace amount of proteins can also be analyzed quantitatively without amplification and labeling in a single cell. Through quantitative analysis of proteins in a single cell level, we can establish new single cell technology and also understand cell-to-cell variation.

Poster Presentation : **LIFE.P-421**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Replication of Methylated DNA Studied with Atomic Force Microscopy

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DNA methylation is one of the epigenetic mechanism that regulates the function of genes without changing the genetic code. It is known that methylated DNA performs not only important genetic roles in normal cells, but also tumor cells. DNA methylation in cancer cells has been observed differently from normal cells, and the degree of DNA methylation of cancer cells are considered to be epigenetic rather than genetic causes. Atomic force microscopy (AFM) have the capability of measuring intermolecular forces at the piconewton level while scanning surfaces at the nanometer resolution. AFM force spectroscopy has been used to observe molecular interaction and dynamics at the single-molecule level. Here, we show a study method of methylated DNA using AFM. In our approach, a DNA polymerase (DNAP) was immobilized on an AFM tip. The DNAP was allowed to capture a duplex of primer/template DNA. Specific rupture events arising from the binding of complementary bases to the DNA/DNAP complex were observed on the nucleotide-immobilized glass slide. Through this study, we propose to identify the differences of DNA methylation during DNA replication process using polymerase and to determine the binding and dissociation constants between the target DNA and its complementary base at the reactive site of the polymerase during the polymerization process. It is expected that the current method would enable the DNA methylation to be studied at the single cell level.

Poster Presentation : **LIFE.P-422**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Giant Unilamellar Vesicles with Actin Polymerization, Mimicry of Cellular Structure

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Mimicking the living cell requires diverse chemical components to handle. First, because the fundamental cellular structure requires cell membrane, we created Giant Unilamellar Vesicles (GUVs) similar sized as living animal cells (10 μ m~100 μ m) as an artificial cellular membrane. We used electroformation for creating GUVs, consisted with the most abundant unsaturated and saturated phospholipids in animal cells, DOPC, DOPS, DPPC, and cholesterol. To mimic the cytoskeletal structure of the cell, we used *Rabbit Skeletal Muscle Actin* for the G-actin, the essential multi-functional protein of all eukaryotic cells, to create actin filaments through actin polymerization. Actin polymerization requires several chemicals to be triggered. It essentially requires divalent cations and ATP. To have a continuous actin polymerization inside the GUVs, it requires the continuous divalent ions supply. As a result, we inserted ionophores (Mg²⁺ and K⁺) in GUVs for the ions supply. We simply encapsulate the G-actin monomers then observed the actin polymerization within GUV, triggered by the change of the Mg²⁺ concentration. These experiments demonstrate the possibility that could lead to the complete artificial creation of living cells structures.

Poster Presentation : **LIFE.P-423**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Antimicrobial activity of quaternary ammonium salt acrylic polymer on various factors.

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Dimethylaminoethylmethacrylate as a tertiary amine and Dimethylsulfate as a cationizing agent were synthesized at a ratio of 1: 1.2, and quaternary ammonium salt was synthesized and used to synthesize an antimicrobial acrylic polymer through acrylate and emulsion polymerization. To confirm the antimicrobial effect on various factors, 70g CCL nonwoven fabric was padded and confirmed by shaking flask method. Factors considered include pick-up amount, quaternary ammonium salt content, and C12 content. First, according to the pick up amount, the higher the pick-up amount, the better the antimicrobial activity. According to one report, the alkyl chain length of the quaternary ammonium salt was changed and the dodecyl compound was found to have the best antibacterial properties. Then, the contents of lauryl methacrylate with C12 were 0%, 10% and 20%, respectively. All of them showed 99.9% antibacterial activity. Finally, the antimicrobial activity of the quaternary ammonium salt was confirmed, and the content of quaternary ammonium salt was 20%, 25% and 30%, respectively. All of them showed 99.9% antibacterial activity.

Poster Presentation : **LIFE.P-424**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Photo-degradation of ERLBD and amyloid fibrils in the presence of ERLBD ligands

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α -Synuclein (α Syn) protein undergoes structural changes to form amyloid fibrils in patients of Parkinson's disease. In our previous study, we examined the process of amyloid fibril formation of α Syn in vitro in the presence of His-tagged ERLBD302-552. In this study, with ERLBD purified we examined the α Syn amyloid formation process through ThT assay in the presence of ligands. We also synthesized a hybrid ligand containing a photosensitizer (2-phenylquinoline) in three steps. Finally, the photo-degradation of ERLBD by the hybrid ligand was observed.

Poster Presentation : **LIFE.P-425**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Assessment of Avian Influenza Virus vs Host-cell Infection Profiling by a Superoxide Detecting Agent (SoDA-1)

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Avian Influenza (AI) virus caused an annual epidemic outbreak that led to destroy millions of poultry, and over 1500 human infection for serious illness or even death. However, studies of AI virus infection in the host have been hampered due to the complex propagation mechanism of the virus, and high rate of mutations during AI replication. In addition, susceptibility of AI virus differs depending on genetic backgrounds of hosts. Till now, research has been carried out for the rapid diagnosis of the viral infection. The existing gold-standard diagnosis method is the culturing of viruses in a chicken embryonated egg for days followed by a hemagglutination assay. Positive samples from this assay is subsequently analyzed by immunoblotting or PCR sequencing to confirm subtypes. This whole method requires specialized facilities to handle large number of pricey embryonated eggs, and costly reagents. Moreover, fast mutation of AI virus leads to antigenic drift that significantly hamper the antibody-based assay. Therefore, a fast and simple surveillance method for AI infection is crucially required. Here, a differential sensing approach to distinguish AI subtypes using cell lines and fluorescent sensors was demonstrated. Different organs originated cell lines might have significantly different susceptibility against AI viruses, since host cells consist of diverse proteins or surface glycan structures. To quantify AI infection, a highly cell-permeable fluorescent sensor was designed, which reacts with superoxide that is an upstream product of AI infection as host cell defense mechanism. This differential sensing strategy successfully proved discriminations of AI subtypes and demonstrated as a useful primary screening platform to monitor a large number of samples.

Poster Presentation : **LIFE.P-426**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Direct observation of DNA substitutive mutations in human cells by CRISPR-Cas9 endonuclease

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CRISPR-Cas9 is used to immune system resisting external plasmid and viruses in prokaryotes by degrading the invading nucleic acids. CRISPR-Cas9 is used for a powerful genome editing tools by taking the function of nuclease. After CRISPR-Cas9 binds the target DNA sequence, CRISPR-Cas9 makes a double-stranded break (DSB) in specific region. The DSB is repaired by non-homologous end joining (NHEJ) and homology directed repair (HDR) systems. HDR recovers the DNA sequence perfectly, but NHEJ can make insertions, deletions and substitutions. The analysis of substitutions is difficult, because the substitutions also can be produced by PCR and next generation sequencing (NGS) error. So, we develop the analysis method for substitution and analyze the pattern of substitutions at 98 samples.

Poster Presentation : **LIFE.P-427**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Sensitive Near-Infrared Fluorescence Probe for H₂O₂ Imaging

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Hydrogen peroxide (H₂O₂) is one of reactive oxygen species (ROS) which play a significant role in aging and the development of chronic diseases such as cancer, stroke, nerve disorder and other. Especially, H₂O₂ is toxic owing to oxidation of proteins, membrane lipids and DNA by the peroxide ion, so detecting H₂O₂ is greatly important for diagnosing various chronic diseases. Up to date, effective methods for imaging H₂O₂ are still lacking though a lot of approach has been reported to detect H₂O₂ in solution. Therefore, it is required to develop a near-infrared (NIR) fluorescent detection probe for H₂O₂. In this study, we designed and synthesized novel NIR probes, NIR hemicyanine skeleton (HXPI) moieties, to detect H₂O₂ in aqueous media. Fluorescence of the NIR probes was enhanced when oxidized from boron group to hydroxyl group by H₂O₂.

Poster Presentation : **LIFE.P-428**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Target-specific Color Development for Food-residential Bacteria Detection by Low-cost 3D Paper Device with Cocktailing Chromogenic Substrates.

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Enzymatic substrate has been regarded as one of powerful tools for quantification and evaluation of bacterial activity. Here, we investigated chromogenic substrates for four strains of pathogenic bacteria, *Escherichia coli*, *Escherichia coli O:157*, *Salmonella spp.*, *Staphylococcus*, with collaborating paper-microfluidic devices. The developed three-dimensional paper sensor consisted of multilayered sheets of wax-patterned paper, cocktailed chromogenic substrates, lysis and oxidation agent. Each mixed enzymatic substrate mixture offered specificity on the target bacterium with showing four-different colors. Without enhancement step, the LOD below 10^8 cfu/mL was demonstrated with 60 min of analysis time. With enhancement treatment for 4 hours, the lower number of bacteria (~ 10 cfu/mL) was detected. When spiked into food sample with enhancement for 8 hours, the specimens were sensitively (10 cfu/mL) detected by image analysis and naked eye observation both. The compact, free-equipment and easy-to-use paper sensor is expected to show utility in first screening detection and quantitative analysis of foodborne pathogen.

Poster Presentation : **LIFE.P-429**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Multi-detectable Bacteria Sensing Device with Color Profiling for Highly Selective Detection of Various Foodborne Pathogens.

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Bacterial pollution of food is one of the public health threat on global. Many kinds of pathogenic bacteria including *Escherichia coli*, *Escherichia coli O:157*, *Salmonella spp.*, *Staphylococcus* can cause deadly food-related illness. To manage these risks, we had previously suggested a point-of-care paper device detecting bacteria with chromogenic substrates. Though it had showed meaningful results, low selectivity among background bacterial strains had been remained as limitation. Here, we developed a high-selective enzymatic paper sensor having four observation sections with chromogenic substrates mixture. Depending on the reaction of each substrate to target bacterium, different colors were represented on the observation regions. RGB analysis of the color reaction showed that each bacterial strain had a specific RGB pattern. This allow us to increase selectivity for background bacterial strains. The compact and easy-to-use paper sensor is expected to show potent utility in qualitative and quantitative analysis of foodborne pathogenic bacteria.

Poster Presentation : **LIFE.P-430**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Construction of non-canonical PAM-targeting adenosine base editors by restriction enzyme-free DNA cloning using CRISPR-Cas9

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Molecular cloning is an essential technique in molecular biology and biochemistry, but it is frequently laborious when adequate restriction enzyme recognition sites are absent. Cas9 endonucleases can induce site-specific DNA double-strand breaks at sites homologous to their guide RNAs, rendering an alternative to restriction enzymes. Here, by combining DNA cleavage via a Cas9 endonuclease and DNA ligation via Gibson assembly, we develop a precise and practical DNA cloning method for replacing part of a backbone plasmid. We first replaced a resistance marker gene as a proof of concept and next generated DNA plasmids that encode engineered Cas9 variants (VQR and VRER), which target non-canonical NGA and NGCG protospacer-adjacent motif (PAM) sequences, fused with adenosine deaminases for adenine base editing (named VQR-ABE and VRER-ABE, respectively). Ultimately, we confirmed that the re-constructed plasmids can successfully convert adenosine to guanine at endogenous target sites containing the non-canonical NGA and NGCG PAMs, expanding the targetable range of the adenine base editing.

Poster Presentation : **LIFE.P-431**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Comprehensive comparison of Cas9 and Cpf1 in human cell

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CRISPR-Cas, an intrinsic immune system of bacteria, has been found in a number of bacterial species, among which two RNA-guided endonuclease, Cas9 and Cpf1, are now widely used as powerful genome editing tools. Because Cas9 and Cpf1 have unique characteristics and need to be compared to which CRISPRs are more suitable for genome editing tools, we chose an endogenous region where both CRISPR systems in human cells can target. In addition, the cleavage regions of two CRISPR were matched to make more clear comparison. We compared the success rate (> 1%), average mutation ratio, indel pattern, and KI efficiency (ssODN, HDR, and NHEJ-mediated K.I) of SpCas9, AsCpf1 and LbCpf1 in these 68 selected endogenous targets. These comprehensive comparisons will allow us to show which CRISPRs are most effective as a genome engineering tool.

Poster Presentation : **LIFE.P-432**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

A Fluorescent Probe for Protein Histidine Phosphatase Activity

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Protein histidine phosphorylation plays an important role in cell signaling and metabolic processes, particularly in bacteria, fungi, and plants. In mammals, protein histidine phosphatase (PHPT1) is one of a few characterized protein phosphatases specific towards phosphohistidine (pHis), and it is shown to regulate the activities of diverse ion channels as well as metabolic proteins. Its activity has been linked to cancer metastasis and diabetes, but further studies have been hampered due to the lack of suitable tools including convenient and accurate phosphatase activity assays. Previous assays relying on a radiolabeling are hazardous and technically laborious. While chromogenic or fluorogenic small molecule substrates have also been used, they are nonselective towards PHPT1 and their kinetic parameters are different from native substrates. To address this, we herein report a fluorescent probe for the pHis activity of PHPT1. With this probe, we conveniently obtained the kinetic parameters of PHPT1 towards a pHis substrate, which showed orders of magnitude difference from the literature values. Our probe was also selective towards PHPT1 over a panel of phosphatases, potentially applicable in monitoring PHPT1 activities in biological samples.

Poster Presentation : **LIFE.P-433**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Structural insight into molecular mechanism of PsnB gained by homology modeling and molecular dynamics simulation

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Plesiocin is recently reported as a new kind of ribosomally-synthesized and post-translationally modified peptides (RiPPs). After a precursor peptide is synthesized by the ribosome, modifying enzyme binds to the leader peptide and builds ester bonds between the specific side chains of the core peptide. Since cyclic peptides are prone to have diverse biological activity, this macrocyclization reaction of PsnB has a possibility to be a versatile tool for biotechnology. In order to understand the molecular mechanism of PsnB, leader truncation experiments and core mutation study were attempted. However, detailed atomic interpretation is still unavailable. Therefore, structural insights were sought to be gained from homology modeling and molecular dynamics simulation. The Galaxy TBM program proposed several amino acid residues as key interacting residues and *in vitro* point mutation experiments are in progress simultaneously. Preliminary mutation study aligned fairly well with the model structure with minor differences to be revised in the model. In addition, molecular dynamics simulation was utilized to discuss the two hypotheses of coupling mechanism: one enzyme-driven folding or the fluctuation-driven folding.

Poster Presentation : **LIFE.P-434**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Biological Cell Fluorescence Imaging with Polymer Dot

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Raman scattering is an emerging contrast mechanism for biological imaging due to its narrow spectral bandwidth. However, the sensitivity is many orders of magnitude lower than that of fluorescence. Fluorescence offers extremely high sensitivity, but suffers from broad absorption and emission spectra. Since Raman and fluorescence are complementary to each other, we developed conjugated polymer-based nanoparticles (Pdots) as an imaging probe for both Raman and fluorescence for cellular imaging. The Raman-active vibrating groups in the Pdots that are electronically resonant to the π -conjugation system produced highly enhanced Raman scattering signals. When the Pdots were irradiated with 532 nm laser near the absorption maximum of the π -conjugated small molecule, the Pdot produced highly enhanced Raman signal for the vibrational modes at 1200-1800 cm^{-1} , while emitting high far-red fluorescence to the sensitivity level of detecting single particles. By conjugating the carboxylic groups on the Pdots and the amine groups on proteins such as avidins and antibodies, we labeled specific proteins in the cell with Pdots and performed molecular-specific cell imaging experiments. Imaging probe with both fluorescence and Raman-activity is a unique and powerful tool that combines high multiplexing of Raman and single-particle sensitivity of fluorescence.

Poster Presentation : **LIFE.P-435**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Supramolecular Proteomic Mapping: Enrichment of Nuclear Proteins by Cucurbit[7]uril-immobilized Beads.

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Enrichment of proteins of interest is one of a key step in proteomic workflow. Currently, chemical labeling of a certain protein/protein family with biotin (Bt) and following enrichment with streptavidin (SA)-conjugated beads are widely used. However, it has inherent limitations such as biomolecular contamination from endogenously biotinylated proteins, damage of proteins in harsh eluting condition. Cucurbit[*n*]urils (CB[*n*]) are emerging macrocyclic molecules which can form host-guest binding pairs with high binding affinity comparable to the Bt-SA pair. We have reported a protein enrichment tool using cucurbit[7]uril (CB[7]) and ferrocenyl- (FcA) or adamantly-ammonium (AdA) as ultrastable host-guest binding pairs. Uses of the CB[7]-conjugated bead enabled us to enrich plasma membrane proteins and intracellular target proteins. To verify CB[7]-based host-guest binding pairs as a versatile proteomics tool, here, we report enrichment of nuclear proteins by combining the CB[7]-bead enrichment system with an enzymatic chemical tag labeling approach (APEX), a spatiotemporal protein labeling method. It enables us to isolate nuclear proteins with minimal biomolecular contamination and conserved spatiotemporal context. By achieving that, this supramolecular tool may become a powerful proteomics tool for isolation and enrichment of almost any protein located in cells, from the plasma membrane to the nucleus.

Poster Presentation : **LIFE.P-436**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Development of ssDNA aptamer for diagnosis and inhibition of highly pathogenic avian influenza virus subtype H5N1

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Avian influenza viruses have devastated the poultry industry in numerous countries irrespective of industrial development resulting in the deaths of millions of birds. Highly pathogenic avian influenza (HPAI) is characterized by high mortality and ability to spread directly from birds to humans. The early diagnosis of avian influenza has been difficult because of its variations in the pathogenicity and the genetic diversity of each virus subtype. Therefore, it is urgent to develop a sensitive and accurate virus diagnosis system. We developed ssDNA aptamer as a small probe to diagnose avian influenza. Through 6 rounds of SELEX towards one of highly pathogenic subtype virus (H5N1), we identified 16 aptamer sequences and selected 2 sequences based on higher frequency. The two selected aptamers showed strong binding affinities and low detection limits. We found that it could bind more specifically to H5N1 compared to other avian influenza virus subtypes. Furthermore, our aptamer inhibited the aggregation of red blood cell which is called hemagglutination. Though more research is needed such as binding site or way of signal translation, our results showed that the screened aptamers worked well as a small molecular probe towards H5N1. It will stand livestock industry in good stead by applying to sensitive diagnosis or suppression of avian influenza.

Poster Presentation : **LIFE.P-437**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Fluorescent Probe for Dynamics of Arginine Phosphorylation

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Protein phosphorylation plays a crucial role in cell signaling and other physiological processes, thus dysregulated phosphorylation has been related to various human diseases. While protein phosphorylations on serine, threonine, and tyrosine have been studied extensively, protein arginine phosphorylation has been less explored because it is incompatible with current phosphoproteomic methods due to its chemical instability. However, recent studies discovered the novel roles of pArg's regulatory function in cells. In gram positive bacteria, pArg was reported to modulate a stress regulator protein (CtsR heat shock regulator). Furthermore, pArg as a protein degradation tag in bacteria recognized by ClpCP protease, suggests that arginine kinases and phosphatase can be novel antibacterial drug targets. Here, we introduce real-time fluorescence based chemosensors to monitor the dynamics of protein arginine phosphorylation and dephosphorylation. These chemosensors enabled continuous measurement of both McsB (protein arginine kinase) and YwIE (protein phosphoarginine phosphatase) activities. Given the growing interest in the protein arginine phosphorylation, mainly in bacteria, we believe this tool will facilitate further understanding of this underappreciated form of protein phosphorylation, paving the way for future drug discovery.

Poster Presentation : **LIFE.P-438**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

The endogenous protein purification in Human cell using CRISPR-Cas

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Production of human protein in different species has clear limitations, such as a cloning problem and an absence of proper protein folding system. In contrary, endogenous human protein exist on low concentration in cells and there is no way to purify a specific protein from extremely heterogenous total proteins. Recent advance of genome editing technology using CRISPR-Cas enable to engineer endogenous genes. We engineered endogenous gene in human cell and purify a huge signal peptide which are secreted. Purified peptides effectively functioned to cells through those known receptors at low dose than its recombinant partial formed peptide which were produced in E.Coli system.

Poster Presentation : **LIFE.P-439**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

CRISPR-Cas9-based strategies to alleviate ABCD1 protein deficiency in X-linked adrenoleukodystrophy

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X-linked adrenoleukodystrophy (X-ALD) is a peroxisomal disease which has variable clinical spectrum and is caused by mutations in the ATP binding cassette subfamily D member 1 (*ABCD1*) gene. *ABCD1* gene encodes ABCD1 protein located in the peroxisomal membrane, and deficiency of ABCD1 protein impairs the peroxisomal beta-oxidation of very long-chain fatty acids (VLCFA). Recently, clustered regularly interspaced short palindromic repeats (CRISPR)-CRISPR-associated protein 9 (Cas9) has been widely studied as it holds potential for therapeutic applications. In this study, we utilized CRISPR-Cas9-based strategies to make genetic background possible to express functional ABCD1 protein in ALD patient-derived fibroblasts cells. ssODN donor or an evolved transfer RNA adenosine deaminase fused to a catalytically impaired CRISPR-Cas9 which is known as adenine base editor (ABE) was used to convert a point mutation(c.796G>A, p.Gly266Arg) into normal. Also, we tried to insert *ABCD1* cDNA encoding normal ABCD1 protein using non-homologous end joining (NHEJ)-mediated knock-in. As a result, we found that the frequency of ABE-mediated gene correction was higher than that of ssODN-mediated gene correction and confirmed the insertion of *ABCD1* cDNA.

Poster Presentation : **LIFE.P-440**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Synergistic Anticancer Effects of the Receptor Tyrosine Kinase Inhibitor Vandetanib and SHP2 inhibitor (Polyphyllin D) on T-cell Acute Lymphoblastic Leukemia Cell Lines

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FDA-approved vandetanib is a small-molecule receptor tyrosine kinase (RTK) inhibitor that is used in cancer treatment. However, resistance to vandetanib can be developed within a few years, resulting in cancer relapse. SHP2 promotes the activation of RAS by regulating signaling upstream of Ras and is a key mediator of programmed cell death 1 and B- and T-lymphocyte attenuator immune checkpoint pathways. Based on the involvement of SHP2 and RTK in cell proliferation, we hypothesized that simultaneous inhibition of SHP2 and RTK could result in a potent anticancer effect overcoming cellular resistance to vandetanib. However, the majority of SHP2 inhibitors suffer from poor selectivity as they also target various other protein tyrosine phosphatases (PTPs), presumably due to the highly conserved active site of PTPs. To search SHP2 inhibitors, we screened 658 phytochemicals to identify many natural product SHP2 inhibitors with strong inhibitory activity, however only polyphyllin D showed inhibitory selectivity to SHP2 over other PTPs although their inhibitory activities are moderate ($K_i = 64.2, 66.5\mu\text{M}$). Furthermore, T-cell acute lymphoblastic leukemia cell lines were treated with vandetanib and the selected SHP2 inhibitors. Combination index values were determined to demonstrate that vandetanib and SHP2 inhibitor show synergistic inhibition of cancer cell growth. Increase in PARP cleavage and caspase-3 activation was observed, meaning that the combination of vandetanib and SHP2 inhibitors induce stronger cancer cell apoptosis in the signal associated with ERK, AKT, Bcl2. Keywords: Vandetanib; receptor protein kinases; SHP2; T-ALL; apoptosis; cancer treatment; synergistic; combined treatment

Poster Presentation : **LIFE.P-441**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Identification of potent and selective natural product inhibitors targeting receptor-type tyrosine-protein phosphatase epsilon (RPTP ϵ) associated with breast cancer

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Receptor-type tyrosine-protein phosphatase (RPTP ϵ) is a classical receptor type PTP encoded by the PTPRE gene. RPTP ϵ is associated with EGFR and ERK1/2 signaling pathway with a positive feedback regulatory loop. It suggests a positive role for RPTP ϵ in cell growth and survival. In human breast cancer cell lines, RPTP ϵ is up-regulated and activated. It indicates up-regulation of RPTP ϵ may contribute to survival of human cancer cell lines. In this study, we have screened phytochemical library consisting of 658-purified single compounds for identifying potent and selective inhibitors of RPTP ϵ . After screening assay, several hit compounds were studied in detail about Ki value and inhibition type. Moreover, we have investigated the efficacy of the inhibitors in human breast cancer cell lines. This study will suggest a valid therapeutic approach for the treatment of cancers.

Poster Presentation : **LIFE.P-442**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Method for identifying lethality of a mutation gene

Se eun Park, Sangsu Bae*

Department of Chemistry, Hanyang University, Korea

CRISPR-Cas system consists of a guide RNA that specifically binds to a specific nucleotide sequence and Cas9 nuclease, which acts as a scissor to cut a specific sequence. By using CRISPR-Cas system, we can make cell lines in which the function of specific genes is knocked out. However, during the course of the experiment, the cell line continued to die during single cell culture, and all the alleles could not continue to obtain the knock-out cell line. The Knock-out cells that died and could not be obtained are due to loss of function of essential genes for survival. Here, we describe the lethality test for cells with knock-out of specific genes, using Next generation sequencing (NGS). Using our method, it can help to know whether the knock-out of a specific gene affects the lethal of the cell, and to avoid repeated experiment failures making knock-out cell line.

Poster Presentation : **LIFE.P-443**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Investigation of natural compounds for cancer treatment through inhibition of PRL-3

Do Hwi Kim, Se Jeong Kwon¹, Ga Hyeon Kim², Hyo Jin Kang³, Sang Jeon Chung^{4,*}

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Protein-tyrosine phosphorylation is a reversible posttranslational modification that is essential for eukaryotic cells. The counteracting activities of protein-tyrosine kinases (PTKs) and protein-tyrosine phosphatases (PTPs) regulate the level of cellular tyrosine phosphorylation. Defective or inappropriate operation of these networks leads to aberrant tyrosine phosphorylation, which contributes to the development of many human diseases including cancers, diabetes, and inflammatory disorders. Phosphatase of regenerating liver-3 (PRL-3) was reported to enhance cell proliferation, motility and invasive activity and to promote cancer metastasis when it was over-expressed. PRL-3 is bound up with cellular process of breast[1], colorectal[2], ovarian[3], prostate[4] and gastric cancers[5]. In present study, several natural products purified from traditional oriental medicinal plants have inhibited PRL-3 expression levels in MCF7 and HCT116 cells. Furthermore, Western blot data of the potent compounds demonstrates its selectivity and possibility to anticancer drugs. Therefore, these inhibitors may be an effective lead compound for the development of anticancer drugs.

Poster Presentation : **LIFE.P-444**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Enhancement antigen binding affinity of scFv-protein nanocage with SpyCatcher/SpyTag system

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²*College of Pharmacy, SungKyunKwan University, Korea*

Single chain variable fragments (scFvs) have potential advantages over whole antibodies, scFvs are one-fifth the size of whole antibodies, they retain antigen binding capacity. It is smaller than IgG but it can binding with antigen and easily make with E.coli system. But scFv 's half-life is shorter than intact, Fc-containing IgG molecule. For exceeding the limit, we use pyruvate dehydrogenase multienzyme complex (PDH). The PDH can self-assembled highly symmetric structure. PDH is composed of 60 subunits, which are self-assembled to form a cage-like nanostructure with external diameter of 23.7 nm[1]. Here we establish a platform for irreversibly conjugating PDHs simply by mixing with protein scFv. We expressed in E. coli PDHs fused to SpyTag and scFv fused to SpyCatcher. SpyCatcher is a genetically-encoded protein designed to spontaneously form a covalent bond to its peptide-partner SpyTag[2]. Using this SpyTag/Catcher system, scFvs have potential advantages over whole antibodies. In this study, we developed the therapeutic potential and safety profiles of high affinity protein nanocage (scFv-PDH) targeted HER2 antigen which are identified using a scFv variant of Trastuzumab and modified PDH. We show that protein nanocage demonstrate high binding affinity and specificity to HER2 antigen.

Poster Presentation : **LIFE.P-445**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Clustering Effect of Interleukin-1 Receptor Antagonist on the Ferritin Nanocage

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Rheumatoid arthritis (RA) is a chronic, autoimmune, inflammatory systemic disease of unknown etiology characterized by persistent joint inflammation that results in progressive joint destruction, joint deformity, and physical disability.¹ Interleukin-1 (IL-1) is one of the pivotal cytokines in initiating and driving the processes of RA. In the body's natural response, IL-1 receptor antagonist (IL-1Ra) has been shown conclusively to block effects of IL-1. However, in presence of the RA synovitis, the induced endogenous production of IL-1Ra is too low to contrast the high affinity of IL-1 for the cell receptors. In this study, clustering of IL-1Ra was used to improve their therapeutic efficacy towards RA. The increased avidity of the IL-1Ra clusters may increase the biological half-life and improve the binding affinity. To this end, IL-1Ra was cloned to the N-terminus of the ferritin monomers and expressed in *E. coli*. Due to the local symmetry of the N-terminus of the ferritin monomers on the surface of the self-assembled nanocage, the IL-1Ras are clustered on the nanocage surface. TEM image of the purified IL-1Ra—ferritin nanoclusters revealed well-formed IL-1Ra—ferritin nanoclusters without any irregular protein aggregates. Also using surface plasmon resonance (SPR), we identified over 50-fold binding affinity of IL-1Ra clusters compared to its monomer.

Poster Presentation : **LIFE.P-446**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Supra-blot: Detection of Proteins Using Ultrastable Synthetic Binding Pairs

Gihyun Sung, Jaehwan Sim¹, Junghyun Kim², Kyunglock Kim³, An Jaeyeon⁴, Sungwan Kim⁵, Hyun-Woo Rhee⁶, Kyeng Min Park^{7,*}, Kimoon Kim^{8,*}

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Modification of proteins with chemical tags has become a promising technique for proteomics by detecting the tags with their binding partners. Biotin has been broadly used as a chemical tag since it is specifically recognized by streptavidin with high binding affinity. A type of western blotting with horseradish peroxidase (HRP) conjugated streptavidin provides detection of the biotin tagged proteins for protein analysis. Although this streptavidin-biotin binding pair is very useful in protein detection, it suffers from various intrinsic problems such as non-desired enzymatic degradation of streptavidin, and unwanted interruption of endogenously existing biotin and biotinylated proteins, causing false positive signals and reduced sensitivity of protein detection. To avoid these problems, here we report a supramolecular chemistry-based protein detection method, termed it as “Supra-blot” using ultrastable synthetic binding pairs, adamantantylammonium (AdA) and cucurbit[7]uril (CB[7]). Specific proteins in bacteria and mammalian cells were labeled with AdA derivatives as chemical tags using various biological means. CB[7]-conjugated horseradish peroxidase (CB[7]-HRP) recognized the AdA-labeled proteins using ultrastable host-guest interactions. The labeled proteins were successfully detected with amplified chemiluminescence signals generated by CB[7]-HRP upon treating H₂O₂ and luminol. These promising

outcomes showed a great potential of the use of Supra-blot for direct detection of AdA-labeled proteins of interest in chemical biology and proteomics.

Poster Presentation : **LIFE.P-447**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Hydroxyapatite-Assisted Enhancement of Subtilisin Activity

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In general, the activity of biocatalyst decreases in organic solvent. Subtilisin (protease from *Bacillus licheniformis*), which is one of the widely used enzymes in industry, also exhibits low activity in organic solvents. However, it has been known that lyophilization of subtilisin with KCl salt dramatically improves subtilisin activity in organic solvents by up to a factor of 100. Although KCl salt is useful to improve subtilisin activity, there are a few drawbacks, such as difficulties of controlling moisture contents and recycling the enzyme, for the application of organic synthesis. In the current study, hydroxyapatite has used as a supporting material for subtilisin immobilization. Hydroxyapatite is one of the main components of the biological bone system, and is non-toxic and biocompatible. A series of the lyophilized forms (2-20%) of subtilisin with hydroxyapatite were prepared and their activities were compared with that of the free form of subtilisin in organic solvents such as hexane, isopropyl ether, and THF. The immobilized subtilisin on hydroxyapatite exhibited the comparable activity to that of the lyophilized form of subtilisin with KCl and can be recycled several times.

Poster Presentation : **LIFE.P-448**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

A novel BODIPY based Chemosensor for Pd (II) ions in live cells.

Kyung Tae Hong, Nicholas Asimwe, Jimin Lee, Dhiraj Murale, Jun-Seok Lee*

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

Palladium has been used in industries due to its specific physicochemical properties, henceforth released in a large amount of residue into the environment. The released Palladium has adverse impact on human health by disturbing various cellular processes by binding with thiol-containing amino acids, proteins, DNA and other macromolecules present inside the cells. Therefore, there is high demands to develop the fluorescent sensor for the palladium ions. In recent years, optical (both colourimetric and fluorometric) technique has emerged out to be the most effective and convenient technique, due to high sensitivity, selectivity, low detection limits and naked-eye detection. Herein, a novel 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) based fluorescence 'turn-off' probe (PdBD-1) have been designed and synthesized for selective detection of palladium(II) (Pd²⁺) ions with a limit of detection (LOD) of 1.66 μ M. The quenching of fluorescence intensity is due to the heavy atom electronic effects of palladium. Using our turn-off probe, we demonstrated Pd²⁺ ions sensing in the live cell imaging application.

Poster Presentation : **LIFE.P-449**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Fast DNA-PAINT Imaging with Reductive Caging

Soohyun Jang, Sang-Hee Shim^{1,*}

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Advances in super-resolution microscopies enable us to observe sub-diffraction-limit organization of biological samples, such as intracellular distribution or structures in cells or tissues. However, super-resolution microscopies have limitations such as photobleaching of fluorescent dyes during prolonged light exposure. DNA-PAINT (Point accumulation in nanoscale topography) overcomes the photobleaching limit by transient binding of short DNAs (docking strands that label the target and imager strands conjugated with fluorescent dye that is complementary to docking strands). The transient binding of short DNAs produces movies of blinking single molecules, resulting in localization-based super-resolution images. However, DNA-PAINT imaging is still limited due to high background from the unbound imaging strands in solution that slows down acquisition speed. To enable fast DNA-PAINT imaging, we combined DNA-PAINT with “reductive caging” in which fluorophores are turned into transient dark states by reducing agents and activated back to the fluorescent state by weak UV illumination. The reduced, caged dyes attached to the imager strands can significantly reduce the background from unbound image strands. Also, an evanescent field of UV can selectively activate caged fluorophores near the substrate, enabling optical control on the turn-on rate. The combination of reductive caging and selective activation can effectively reduce the image acquisition time in a controllable manner.

Poster Presentation : **LIFE.P-450**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Expression and characterization of a novel carbohydrate esterase *SmAcE1* from *Sinorhizobium meliloti* suitable for biodiesel synthesis.

Ly Thi Huong Luu Le, Doo Hun Kim*

Department of Chemistry, Sookmyung Women's University, Korea

Biocatalytic synthesis is a promising environmentally friendly process for the production of biodiesel, a sustainable alternative fuel from renewable plant resources. Here, *SmAcE1* from *Sinorhizobium meliloti*, a gram-negative nitrogen fixing soil bacteria, was identified, purified, characterized and used for synthesis of biodiesel products. *SmAcE1* belonged to an α/β hydrolase fold in GDSL superfamily with catalytic triad Ser15, His195 and Asp192 and oxyanion hole-forming SGNH (Ser15, Gly57, Asn97 and His195). This enzyme was most active at pH 8.0 and it was stable up to 70°C. *SmAcE1* exhibited broad substrate specificity toward various *p*-nitrophenyl esters, lipids, carbohydrates and tertiary alcohols. Furthermore, *SmAcE1* not only synthesized butyl acetate and ethyl acetate but also synthesized different types of oleates by esterification using oleic acid and short chain alcohols (methanol, ethanol and butanol). Therefore, *SmAcE1* might be a good biocatalyst in ester synthesis in biodiesel industry.

Poster Presentation : **LIFE.P-451**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Characterization of a novel penicillin-binding protein from *Lactobacillus acidophilus* NCFM

Ly Thi Huong Luu Le, Doo Hun Kim*

Department of Chemistry, Sookmyung Women's University, Korea

A novel penicillin-binding protein, *LaPBP* from *Lactobacillus acidophilus* NCFM, which is composed of 364 amino acids with a molecular mass of 41 kDa, was identified, expressed and characterized. *LaPBP* displayed a significant sequence similarity with 1SDE, a hydrolases from *Streptomyces* strain R61. Further sequence analysis of *LaPBP* revealed a conserved of S-X-X-K motif and a putative catalytic triad of Ser85-Lys88-Tyr174. *LaPBP* hydrolyzed short-chain esters such as *p*-nitrophenyl acetate, butyrate. Finally, β -lactamase activity of *LaPBP* was investigated. Taken together, this study will contribute to improve our understanding, providing useful information in sequence, biophysical properties and catalytic activity into penicillin-binding proteins family.

Poster Presentation : **LIFE.P-452**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

**Molecular characterization of a novel family V esterase form
Lactobacillus acidophilus NCFM**

Ly Thi Huong Luu Le, Doo Hun Kim*

Department of Chemistry, Sookmyung Women's University, Korea

A novel esterase, *LaEst*, was identified from *Lactobacillus acidophilus* NCFM. The enzyme consisted of 247 amino acids and the molecular mass of *LaEst* was estimated to be 27,369 Da. *LaEst* displayed a significant sequence similarity with LJ0536, a serine cinnamoyl esterase produced by the probiotic bacterium *Lactobacillus johnsonii* N6.2. Further sequence analysis of *LaEst* revealed a conserved pentapeptide of G-X-S-X-G and a putative catalytic triad of Ser106-Asp197-His225. *LaEst* preferred p-nitrophenyl butyrate as a substrate and showed its maximum activity at pH 8.0. In addition, *LaEst* efficiently hydrolyzed α -D-glucose pentaacetate and glyceryl tributyrates. Taken together, this work might provide some useful information in sequence, biophysical properties and catalytic activity of family V esterase.

Poster Presentation : **LIFE.P-453**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

**Crystal structure and functional characterization of a novel FAH
(fumarylacetoacetate hydrolase) family hydrolase from
*Exiguobacterium antarcticum DSM***

Wanki Yoo, Doo Hun Kim^{1,*}

College of Medicine, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

A novel hydrolase, *EaD30* from psychrophilic bacteria, *Exiguobacterium antarcticum DSM* were identified and characterized. Multiple sequence alignment with the sequences retrieved from PSI-BLAST revealed that *EaD30* belongs to FAH (fumarylacetoacetate hydrolase) family. Genetic analysis of *EaD30* locus confirmed that neighboring genes including *EaD30* gene were highly conserved across *Exiguobacterium* strains indicating that *EaD30* has an important role for the strains. Previously, few FAHs were identified and crystallized. Sequence alignment and the crystal structure of the FAHs showed that putative catalytic site, His and Glu, were well conserved and located in a HxxE motif in the lid domain. However, the catalytic lid domain is missing in most crystal structures of the native FAHs, making it hard to elucidate molecular mechanism of catalysis by FAHs. Here, we report the crystal structure of *EaD30*. In the crystal structure of *EaD30*, the catalytic lid domain was well defined without any stabilization by substrates. Furthermore, biochemical and biophysical characters of *EaD30* were studied using spectrofluorometry, circular dichroism (CD), non-denaturing PAGE, and gel filtration chromatography. Collectively, the structure of *EaD30* and biochemical results will pave a way to explain the role of the catalytic lid domain in the catalysis of FAHs

Poster Presentation : **LIFE.P-454**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Characterization of a novel GDSL family lipase (*NmLip*) from *Neisseria meningitidis* 053442

Wanki Yoo, Doo Hun Kim^{1,*}

College of Medicine, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Family II lipases, also known as GDSL family lipases, exhibit a broad substrates specificity hydrolyzing carbohydrates, tertiary alcohol esters, and lipids. GDSL family lipases have a typical α/β hydrolase folding and catalytic triads which are generally found in bacterial lipases/esterases. In contrast to esterases, lipases generally have hydrophobic exterior characteristic displaying hydrophobic amino acids on their surface. This property of lipases facilitates the catalysis of lipids at oil-water boundary. Here, *NmLip*, a novel GDSL family lipase from *Neisseria meningitidis* 053442 was identified, purified, and characterized by biochemical and biophysical methods. Homology searching found that *NmLip* shows high sequence similarity to TesA, an *E. coli* lipase belonging to GDSL family. The results of site-directed mutagenesis and molecular simulation revealed that hydrophobic amino acid, Leu92 near the catalytic pocket play a critical role for *NmLip*'s hydrolase activity and substrate specificity through hydrophobic interaction and steric hinderance. As last, immobilization by cross-linking and enzyme-inorganic hybrid nanoflower (hNF) were applied to *NmLip* which have shown a good durability after repeated usages and an improved catalytic efficiency. Collectively, these studies provide a deeper insight to substrate specificity of GDSL family lipase and emphasize potential of *NmLip* as a biocatalyst in the pharmaceutical and chemical industries.

Poster Presentation : **LIFE.P-455**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

Structure and characterization of a novel family VII carbohydrate esterase from *Paenibacillus sp. R4*.

Wanki Yoo, Doo Hun Kim^{1,*}

College of Medicine, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Carbohydrate esterases (CEs) catalyze acetylation and de-acetylation of carbohydrates ranging from simple compounds such as a glucose and mannose to complex polysaccharide like cellulose and xylan. The modifications of carbohydrates are necessary for various application field, such as a polishing of fabric, a preparation of biofuels and highly valuable industrial materials. A cold-active enzyme or a cold-adapted enzyme implies an ambiguous group of enzymes which are usually derived from psychrophilic bacteria. The enzymes present its optimal activity at low temperature indicating the superior structural stability of the enzymes. In this study, *PbAcE*, a novel cold-active family VII carbohydrate esterase derived from *Paenibacillus sp. R4* was identified, purified and crystalized. *PbAcE* was found to have a broad substrate specificity including tertiary alcohol esters, antibiotics related compounds, lipids as well as carbohydrates. Collectively, the crystal structure and biochemical study of *PbAcE* will provide molecular basis of enzyme reaction for both a carbohydrate esterase and a cold-active enzyme

Poster Presentation : **LIFE.P-456**

Life Chemistry

Grand Ballroom, FRI 11:00~12:30

New insights into the chemistry of biological systems studied by ^{17}O NMR at 35.2 Tesla and molecular dynamics and quantum calculations

Myunggi Yi

Department of Biomedical Engineering, Pukyong National University, Korea

Due to the broad linewidths of quadrupolar nuclei, in particular, ^{17}O NMR application to biological systems has been limited. However, recent development in NMR spectroscopy at 1.5 GHz using a 35.2 tesla hybrid magnet improved ^{17}O sensitivity and showed much narrower linewidths. To illustrate that new insights into the chemistry of biological systems can be observed with ^{17}O spectroscopy, spectra of single site ^{17}O labeled gramicidin A in liquid crystalline lipid bilayers have been recorded. While this monovalent cation selective channel has been characterized at high resolution by multiple technologies and labs, it has always been observed to be a symmetric dimer in the absence of ions until 35.2 T ^{17}O spectroscopy showed that the symmetry is broken. Possible explanations due to water distribution in the channel pore studied by molecular dynamics simulations and quantum calculations will be discussed.

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

Organic Chemistry

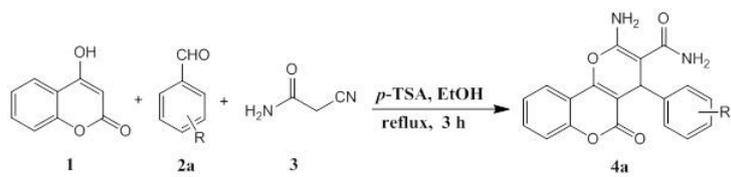
Grand Ballroom, THU 11:00~12:30

A metal-free C–C/C–O bond formation for the synthesis of 2-amino-5-oxo-4-aryl-4H,5H-pyrano[3,2-c]chromene-3-carboxamide catalyzed by p-toluenesulfonic acid (p-TSA)

Yeon Tae Jeong^{*}, Amol Jadhav

Department of Display Engineering, Pukyong National University, Korea

An efficient and eco-friendly procedure for the synthesis of 2-amino-5-oxo-4-aryl-4H,5H-pyrano[3,2-c]chromene-3-carboxamide has been developed through a one-pot three-component condensation of 4-hydroxycoumarin with aldehydes and cyanoacetamide, in the presence of catalytic amount of p-toluenesulfonic acid (p-TSA) as a highly active acid catalyst in EtOH conditions at 80 °C. This new procedure offers several advantages such as shorter reaction times, excellent yields, a wide range of functional group tolerance, easy experimental work-up procedure, operationally simple under metal-free reaction conditions and C-C/C-O bond formation. This procedure useful for the synthesis of heterocyclic compounds.



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

Organic Chemistry

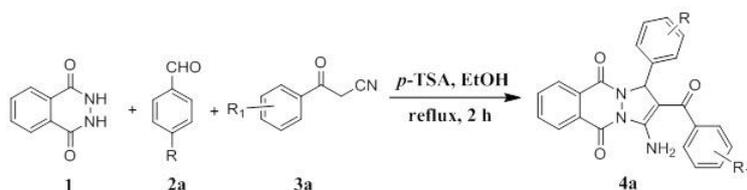
Grand Ballroom, THU 11:00~12:30

A novel three-component method for the synthesis of 3-amino-2-benzoyl-1-aryl-1H-pyrazolo[1,2-b]phthalazine-5,10-dione using p-TSA as a catalyst

Yeon Tae Jeong*, Amol Jadhav

Department of Display Engineering, Pukyong National University, Korea

A convenient, environmentally friendly and efficient procedure for the synthesis of novel 3-amino-2-benzoyl-1-aryl-1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivatives have been developed by one-pot three-component condensation reaction of phthalhydrazide, aldehydes and benzoylacetonitrile in the presence of catalytic amount of p-toluenesulfonic acid (p-TSA) as a acid catalyst in EtOH at 80 °C conditions. This new protocol offers an environmental acceptability, shorter reaction time, low cost, high yields, a wide range of functional group tolerance, simple and easy experimental work-up procedure.



Poster Presentation : **ORGN.P-40**

Organic Chemistry

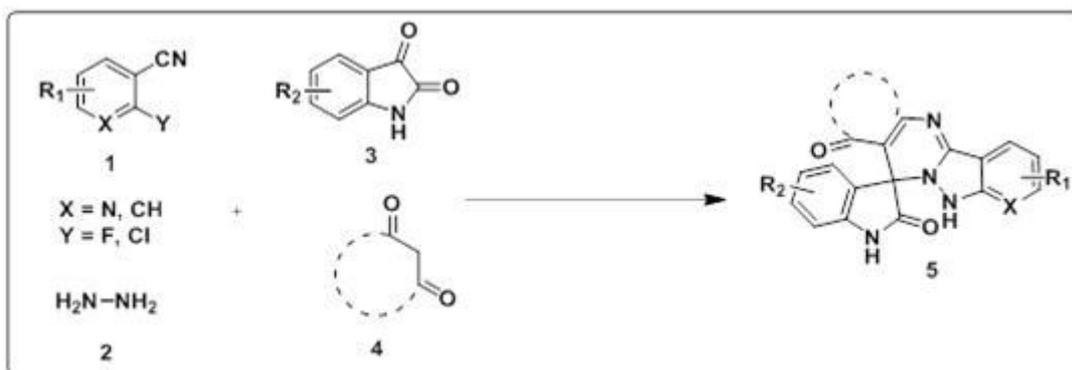
Grand Ballroom, THU 11:00~12:30

Acid-Mediated One-pot Four-Component Process for the Synthesis of Novel Spiro[indazolo[3,2-b]quinazolines: A Green Approach

Yeon Tae Jeong*, Sandip gangadhar Balwe

Department of Display Engineering, Pukyong National University, Korea

A simple and efficient tandem route to novel spiro[indazolo[3,2-b]quinazolines has been developed. The reaction proceeds via in situ generation of the 1H-indazol-3-amines in ethanol followed by its reaction with the cyclic 1,3-dicarbonyls and isatin derivatives to assemble a novel N-fused polyheterocycles. The main advantages of this protocol include short reaction time, excellent yield, easy work-up, operational simplicity and the absence of extraction and chromatographic purification steps.



Poster Presentation : **ORGN.P-41**

Organic Chemistry

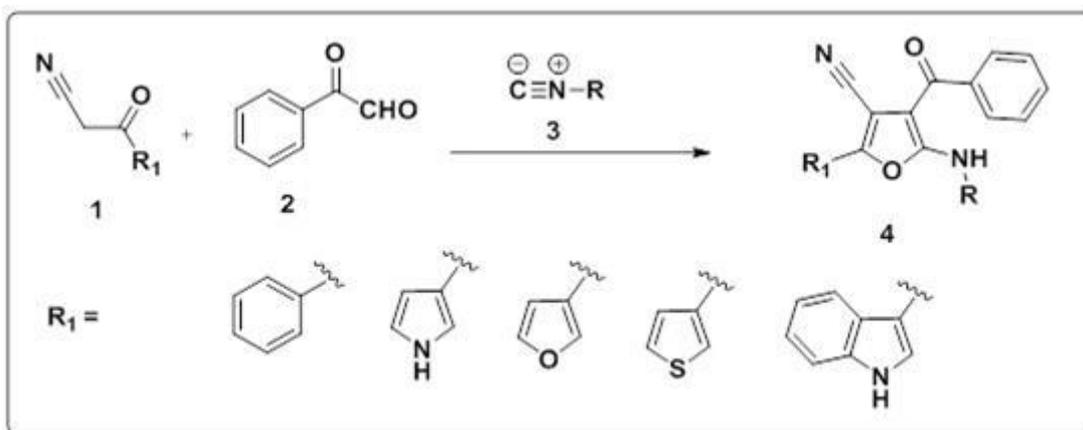
Grand Ballroom, THU 11:00~12:30

Acid-Promoted “One-pot” Tandem Cyclization to Synthesize Densely Functionalized Furans

Yeon Tae Jeong*, Sandip gangadhar Balwe

Department of Display Engineering, Pukyong National University, Korea

A practical, convenient, and cheap method has been explored for the synthesis of densely functionalized furans. This one-pot process involved reaction of aryl glyoxals, isonitriles and series of aromatic and hetero aromatic β -ketonitriles to provide diverse collections of products. Utilizing this synthetic protocol, a variety of polysubstituted furans could be easily obtained in good to excellent yields with different substituted patterns.



Poster Presentation : **ORGN.P-42**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Triazine and pyrimidine based bipolar host materials for highly luminescent green phosphorescence OLEDs

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Department of Chemistry, Wonkwang University, Korea

¹*Wonkwang University, Korea*

In this study, we have designed and synthesized two bipolar host materials namely, 4-(2-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazol-9-yl)-N,N-diphenylaniline (TRZ 1) and 4-(2-(4,6-diphenylpyrimidin-2-yl)-9H-carbazol-9-yl)-N,N-diphenylaniline (PYR 1) for green phosphorescence OLEDs. The triplet energies of PYR 1 and TRZ 1 were 2.63 and 2.44 eV, respectively. Which facilitated proper energy transfer from host to dopant to enhance the efficiencies. The PYR 1 based green OLED device showed maximum current efficiency of 48.7 cd/A with an outstanding brightness of 95,870 cd/m². The brightness value was three times higher than that of CBP based reference green OLED. The external quantum efficiency of PYR 1 based device was 16.4% while TRZ 1 showed 15.4%. Overall performance of pyrimidine based PYR 1 was found as better when compare to CBP and TRZ 1.

Poster Presentation : **ORGN.P-43**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

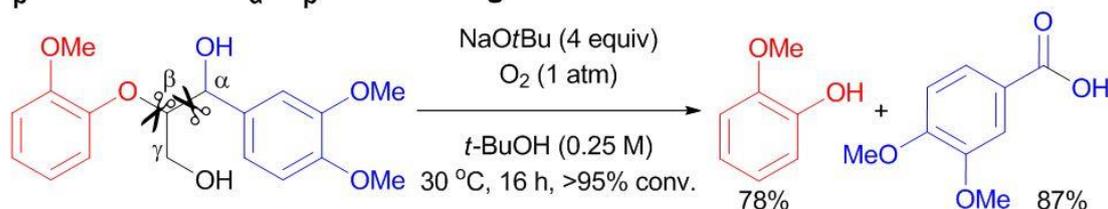
Transition-metal-free conversion of lignin model compounds to high-value aromatics: scope and chemoselectivity

Tae Woo Lee, Jung Woon Yang*

Department of Energy Science, Sungkyunkwan University, Korea

An efficient and straightforward reaction protocol for the conversion of lignin model compounds was developed, based on a simple system consisting of a base, oxygen, and green solvent under mild conditions in the absence of metals. This protocol was successfully applied to the cleavage of both 'β-O-4' dimeric and trimeric compounds, and a controlled selective degradation was achieved depending on the bond type. The feasibility of this method to provide aromatic compounds in high yields from lignin by sequential oxidative dehomologation reaction was clearly demonstrated.

C_β-O bond and C_α-C_β bond cleavage



- Transition-metal-free version
- Unprecedented cleavage pattern and product formation
- No requirement of pre-functionalization of substrate
- 22 examples

Poster Presentation : **ORGN.P-44**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Acridine based efficient hole transporting and injecting material for green phosphorescence OLEDs

Braveenth Ramanaskanda, Gyu Youn Chea^{*}, Leero Lee, Hasu Jung¹, Bo Mi Kim

Department of Chemistry, Wonkwang University, Korea

¹Organic Chemistry, Wonkwang University, Korea

We have designed and synthesized acridine-triphenylamine based hole transporting material 4-(9,9-diphenylacridin-10(9H)-yl)-N-(4-(9,9-diphenylacridin-10(9H)-yl) phenyl)-N-phenylaniline (TPA-1A) for phosphorescence OLED applications. TPA-1A exhibited excellent thermal stabilities, with a higher decomposition temperature of 474 oC at 5 % weight reduction. To investigate the hole transporting and injecting properties, green PhOLED was fabricated with TPA-1A and device performances were compared with well-known NPB based similar device. The current efficiency was 44.29 cd/A which is higher than that of NPB based reference device (33.38 cd/A). TPA-1A as hole injecting layer device showed an outstanding power and external quantum efficiencies of 32.37 lm/W, 14.59 %, respectively. TPA-1A based device revealed outstanding device efficiencies when compare to reference NPB based device.

Poster Presentation : **ORGN.P-45**

Organic Chemistry

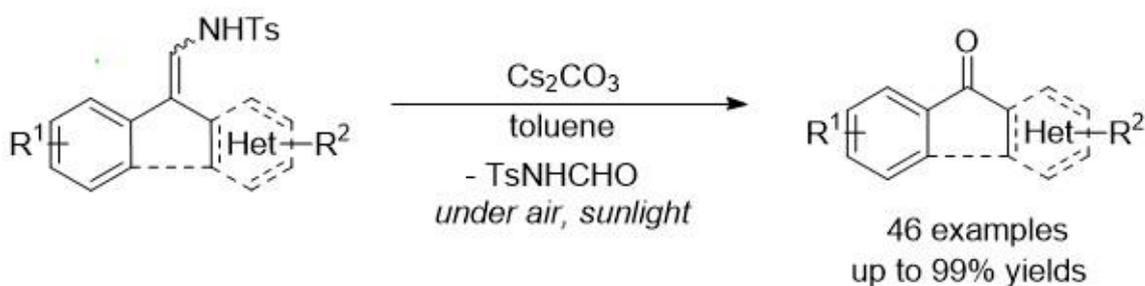
Grand Ballroom, THU 11:00~12:30

Synthesis of Diaryl Ketones *via* Oxidative Cleavage of the C–C Double Bonds in *N*-Sulfonyl Enamides

Gi Uk Han, Gi Hoon Ko, Chanyoung Maeng, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

An oxidative cleavage of C–C double bond is developed from photochemical [2 + 2]-cycloaddition of diaryl *N*-tosyl enamides, aryl heteroaryl *N*-tosyl enamides, and *N*-tosyl cyclic enamides with singlet molecular oxygen followed by ring-opening reaction mediated by Cs₂CO₃ under air and sunlight without the use of photosensitizer, producing symmetrical and unsymmetrical diaryl, heterodiaryl, and cyclic ketones in good to excellent yields. Moreover, the oxidative cleavage of C–C triple bonds from 1-alkynes is demonstrated for the synthesis of symmetrical and unsymmetrical ketones from Cu-catalyzed [3 + 2]-cycloaddition, Rh-catalyzed alkoxyarylation, photooxygenation, and ring-opening reaction in one-pot. Because synthesis of the symmetrical and unsymmetrical diaryl and/or heterodiaryl ketones bearing an electron-donating group is not easy, the present method is notable.



Poster Presentation : **ORGN.P-46**

Organic Chemistry

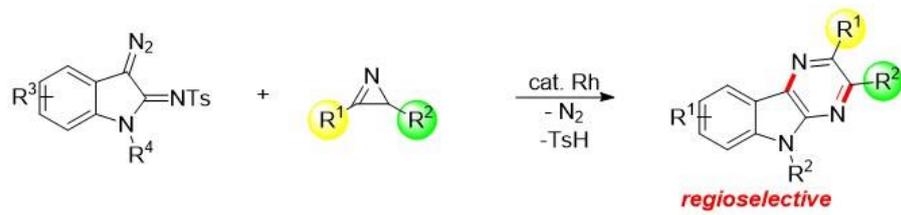
Grand Ballroom, THU 11:00~12:30

Regioselective Synthesis of Indolopyrazine Derivatives through Sequential Rh-Catalyzed Formal [3 + 3] Cycloaddition and Aromatization Reaction of Diazoindolinimines with Azirines

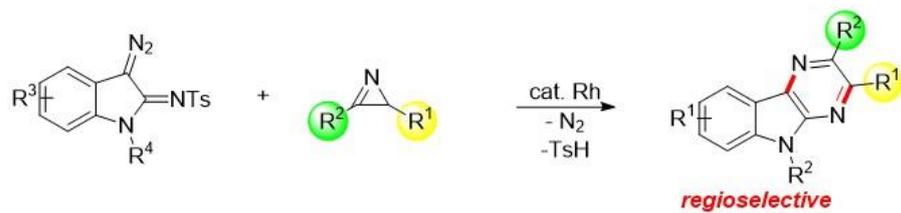
Sang Hoon Han, Gi Hoon Ko, Chanyoung Maeng, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Indolopyrazines possessing both indole and pyrazine moieties are significant structural motifs in a number of naturally occurring products, show a wide range of biological activities, including antitumor and antiviral activities, and function as fluorescent and host materials. In this regard, the indolopyrazine motif has continuously received the attention of synthetic chemists. Thus, establishing synthetic approaches for preparing regioselective indolopyrazines from simply attainable starting materials is highly demanded. We developed a regioselective synthetic method to prepare indolopyrazines through a sequential Rh-catalyzed formal [3 + 3] cycloaddition and aromatization reaction of a wide range of diazoindolinimines with azirines. Because the previously reported synthetic methods afforded mixtures of indolopyrazines, the present method using unsymmetrical azirines has the an excellent merit from a regioselectivity standpoint. Because indolopyrazines are fluorescent, their optical properties in CH₂Cl₂ solution were studied. The extinction coefficients were variable from 107,298 to 585,478 M⁻¹cm⁻¹. The indolopyrazine affords high quantum yields and extinction coefficients, which are an attractive property for biological probes.



36 examples
up to 97% yields



Poster Presentation : **ORGN.P-47**

Organic Chemistry

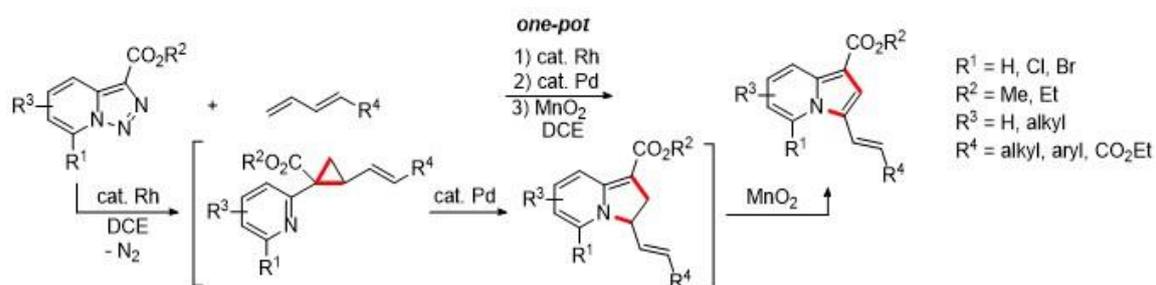
Grand Ballroom, THU 11:00~12:30

One-Pot Synthesis of Indolizines via Sequential Rh-Catalyzed [2 + 1]-Cyclopropanation, Pd-Catalyzed Ring Expansion, and Oxidation Reactions from Pyridotriazoles and 1,3-Dienes

Suhui Kim, Gi Uk Han, Eunchong Jeong, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Development of synthetic methods for accessing a variety of functionalized *N*-heterocyclic compounds is a significant objective in the fields of organic and medicinal chemistry. Because indolizine derivatives containing nitrogens at their ring junction have been found in a number of natural products, pharmaceuticals, and bioactive compounds, the development of expeditious approaches for the construction and functionalization of indolizine derivatives has gained much attention. However, 3-(alkenyl)indolizine derivatives, a vital skeleton for building phosphoinositide 3-kinase inhibitors, have rarely been reported. For this reason, we developed a one-pot synthetic route to 3-(alkenyl)indolizine derivatives via sequential Rh-catalyzed [2 + 1]-cyclopropanation, Pd-catalyzed ring expansion, and oxidation reactions from pyridotriazoles and 1,3-dienes.



Poster Presentation : **ORGN.P-48**

Organic Chemistry

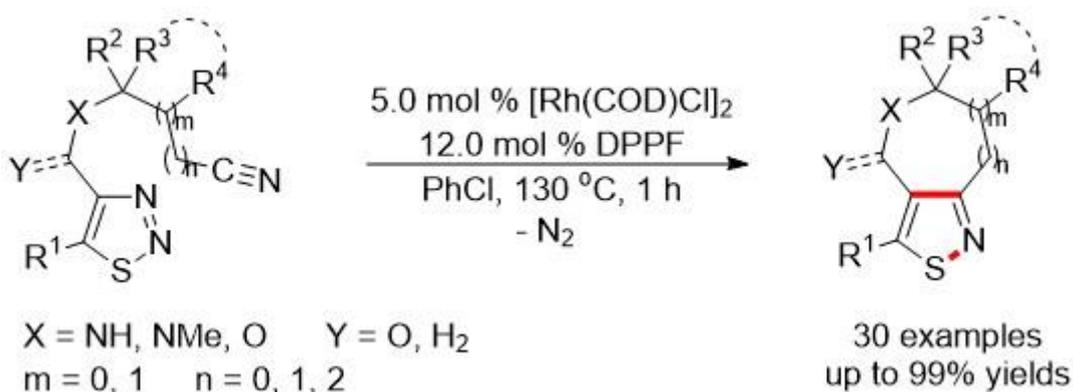
Grand Ballroom, THU 11:00~12:30

Synthesis of Bicyclic Isothiazoles from an Intramolecular Rh-Catalyzed Transannulation of Cyanothiadiazoles

Haeun Jang, Sang Hoon Han, Eunchong Jeong, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Bicyclic isothiazole ring systems are privileged structural motifs found in many pharmaceutical compounds and functional materials. They have been widely used as significant privileged scaffolds in a myriad of areas such as organic electroluminescent materials, semiconductors, pesticides, anticancer drugs, and ligands. Thus, development of an efficient synthetic method for functionalized bicyclic isothiazoles is highly desired. Therefore we developed an intramolecular Rh(I)-catalyzed transannulation of readily available cyanothiadiazoles containing an ester, amide, or ether as a linker, serving as an efficient platform for the construction of a wide range of bi-, tri-, and tetracyclic isothiazoles in good to excellent yields together with the release of molecular nitrogen. These results suggest that the carbon atom in the α -thiavinyl carbene is nucleophilic and that the sulfur atom is electrophilic.



Poster Presentation : **ORGN.P-49**

Organic Chemistry

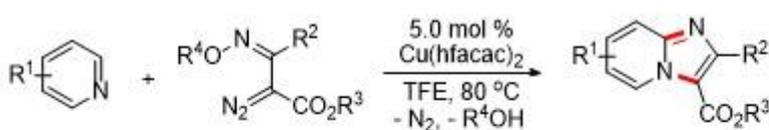
Grand Ballroom, THU 11:00~12:30

Synthesis of Imidazopyridines from Copper-Catalyzed, Formal Aza-[3 + 2] Cycloaddition Reaction of Pyridine Derivatives with α -Diazo Oxime Ethers

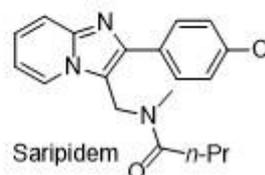
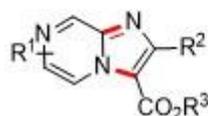
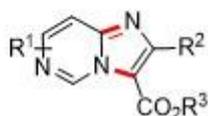
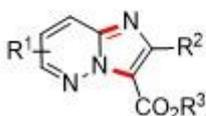
Seung Jin Jung, Dahee Park, Haeun Jang, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

N-Containing heterocyclic compounds are extremely important in the study of biological activity and for pharmaceutical utilization. Especially, imidazopyridines with both pyridine and imidazole moieties, which comprise a typical, privileged scaffold, exhibit gastroprotective properties and function as sedative, anxiolytic, and insomnia medicine. For this reason, the development of a synthetic method for imidazopyridine and its derivatives from easily accessible compounds is needed. So we developed a Cu-catalyzed, formal aza-[3 + 2] cycloaddition reaction with pyridine derivatives and α -diazo oxime ethers in trifluoroethanol to synthesize imidazopyridines with the release of molecular nitrogen and elimination of alcohol. This method enabled modular synthesis of a wide range of N-heterobicyclic compounds such as imidazopyridazines, imidazopyrimidines, and imidazopyrazines.



- ☑ Simple conditions
- ☑ Easy handling
- ☑ Cheap Cu catalyst
- ☑ Modular synthesis



Poster Presentation : **ORGN.P-50**

Organic Chemistry

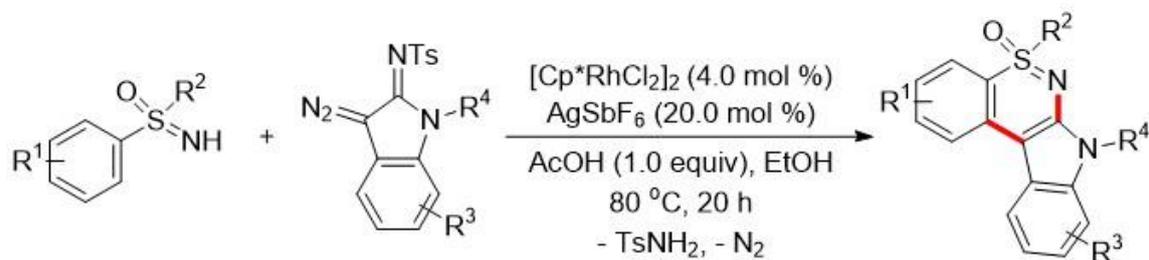
Grand Ballroom, THU 11:00~12:30

Synthesis of Indolo-1,2-benzothiazine Derivatives *via* Sulfoximines and 3-Diazoindolin-2-imines

Jinhui Won, Dae Kyum Kim, Suhui Kim, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Sulfoximines are significant compounds that are found in pharmaceuticals, bioactive compounds, and agrochemicals. Accordingly, the development of novel synthetic methods for sulfoximines and their modifications have become highly attractive. To date, many synthetic methods using these tools have been reported in the literature. These methods have focused mainly on the preparation of linear sulfoximines and their derivatives. However, synthetic approaches for the construction of cyclic sulfoximines have been relatively limited. We developed a novel synthetic method for indolo-1,2-benzothiazines *via* the Rh-catalyzed cyclization of *S*-aryl sulfoximines with 3-diazoindolin-2-imines together with the release of molecular nitrogen and *p*-toluenesulfonamide. The present method involved the N-H/C-H activation of *S*-aryl sulfoximines. A wide-ranging scope of both *S*-aryl sulfoximines and 3-diazoindolin-2-imines was demonstrated.



Poster Presentation : **ORGN.P-51**

Organic Chemistry

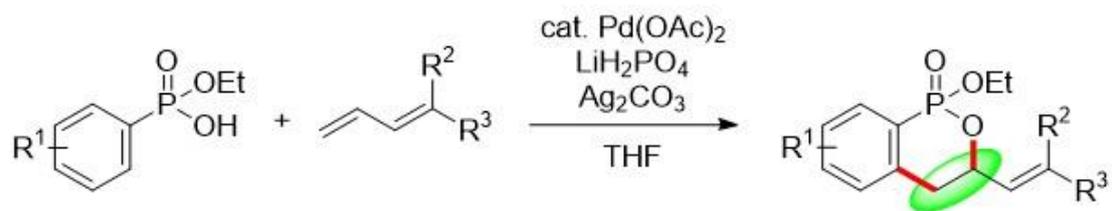
Grand Ballroom, THU 11:00~12:30

Synthesis of Dihydrophosphaisocoumarins through a Palladium-Catalyzed Oxidative Cyclization of Arylphosphonic Acid with 1,3-Dienes

Yongjoo Yun, Kyungsup Lee, Seung Jin Jung, Phil Ho Lee*

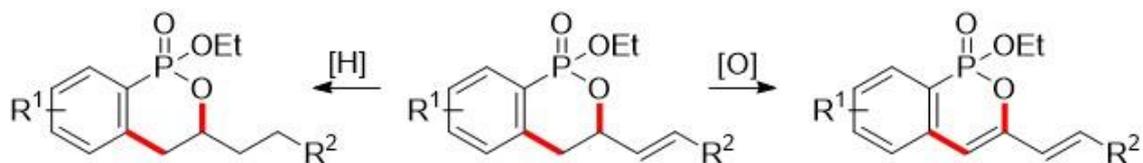
Department of Chemistry, Kangwon National University, Korea

Organophosphorus compounds are an omnipresent structural motif found in living organisms and biologically active compounds, and their facile synthesis is important in the preparation of synthetic intermediates, agrochemicals, and pharmaceuticals. Additionally, these compounds have continuously attracted great interest due to their role as bioisosteres of carbonyl and carboxylate groups. Accordingly, much effort has been devoted not only to construct skeletons of phosphorus compounds but also to introduce new functional groups onto these compounds. However, in contrast their acyclic analogs, the synthesis and application of phosphaheterocyclic compounds have been rarely investigated. We developed an efficient synthetic method for the selective preparation of dihydro-phosphaisocoumarins and their derivatives through a Pd-catalyzed oxidative cyclization reaction of a wide range of arylphosphonic acid monoethyl esters with activated and unactivated 1,3-dienes, including 1-aryl-substituted 1,3-dienes and 1-alkyl-substituted 1,3-dienes, thus opening a new avenue for the synthesis of phosphaheterocyclic compounds.



R^1 = alkyl, aryl, halide

R^2, R^3 = alkyl, aryl, electron-withdrawing group



Poster Presentation : **ORGN.P-52**

Organic Chemistry

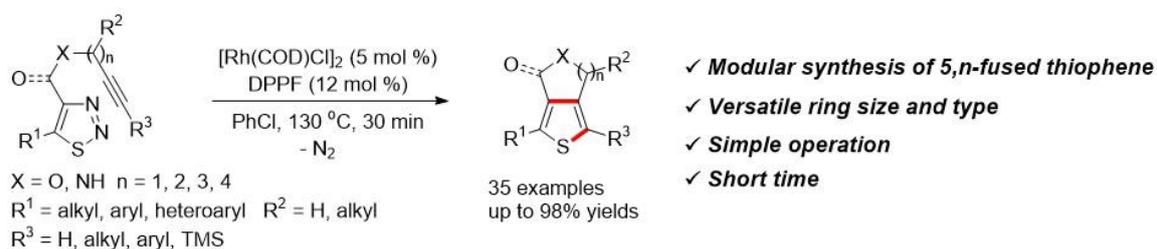
Grand Ballroom, THU 11:00~12:30

Synthesis of 5,*n*-Fused Thiophenes through Rhodium-Catalyzed Intramolecular Transannulation Reaction of Alkynyl Thiadiazole

Kyungsup Lee, Gi Uk Han, Chanyoung Maeng, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Fused thiophenes have been recognized as very important scaffolds in the field of pharmaceutical and functional materials sciences. For this reason, the development of an efficient synthetic method for functionalized fused thiophenes is highly attractive and poses a significant challenge. However, because some of the previously reported synthetic methods demand a strong base, long reaction times, and vigorous reaction conditions, the development of efficient synthetic approaches to overcome these shortcomings has been continuously required. Herein, we developed a method for the synthesis of a wide range of fused thiophenes, including those fused with lactams, lactones, or cyclic ethers, from a rhodium-catalyzed intramolecular transannulation reaction of alkynyl thiadiazoles. This transannulation reaction provides an efficient platform for the construction of a variety of 5,*n*-fused thiophenes from readily available starting materials together with the release of molecular nitrogen.



Poster Presentation : **ORGN.P-53**

Organic Chemistry

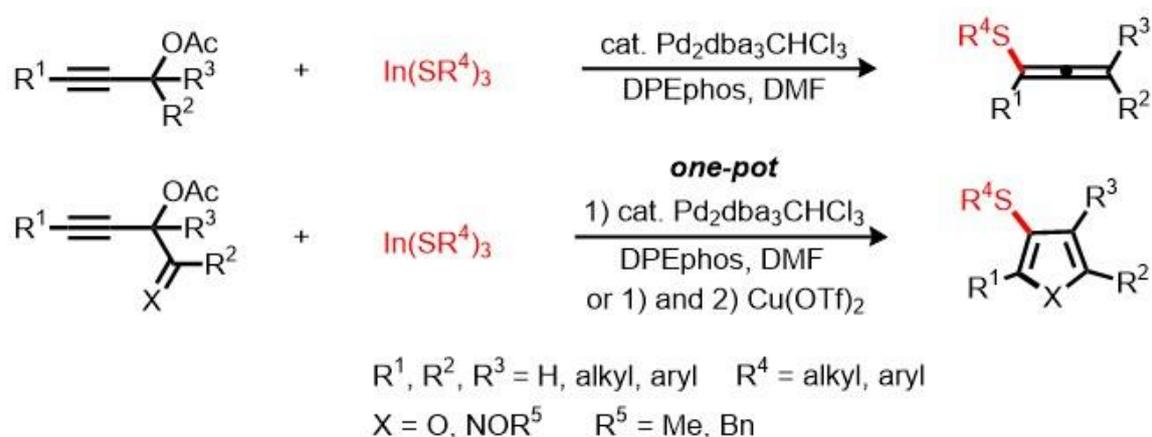
Grand Ballroom, THU 11:00~12:30

Synthesis of Multisubstituted Allenes, Furans, and Pyrroles *via* Palladium-Catalyzed Substitution and Cycloisomerization in one pot

Dae Kyum Kim, Sang Hoon Han, Jinhui Won, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Recently, an efficient synthetic method towards multisubstituted furans and pyrroles bearing hetero-substituents was reported through metal-catalyzed 1,2-shifts of diverse migrating groups in allenyl systems. However, the introduction of a wide variety of substituents at the 4-position of furans and pyrroles is impossible due to requirement of [1,3]-H shift in these methods. Therefore, the development of an efficient synthetic method for multisubstituted furans and pyrroles bearing 3-heteroatom substituents as well as substituents at the 4-position has been a continuing challenge. Herein, we report Pd-catalyzed propargyl substitution reactions of propargyl acetates with indium organothiolates for the synthesis of multisubstituted allenyl sulfides. This procedure employed tandem Pd-catalyzed propargyl substitution and cycloisomerization reactions from indium organothiolates and propargyl acetates bearing acyl and imidoyl groups for the synthesis of multisubstituted furans and pyrroles in one-pot.



Poster Presentation : **ORGN.P-54**

Organic Chemistry

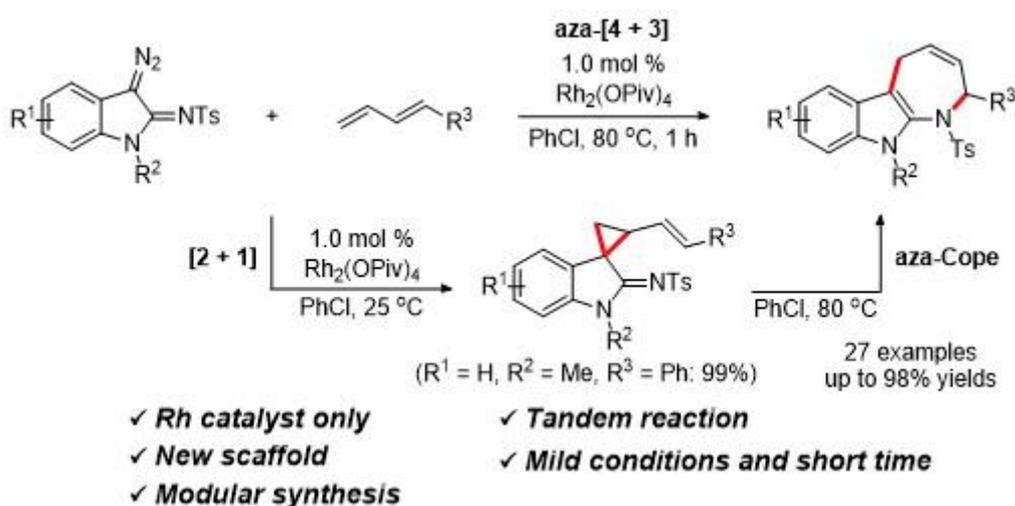
Grand Ballroom, THU 11:00~12:30

Synthesis of Azepinoindoles *via* Rh-Catalyzed Formal Aza-[4 + 3] Cycloaddition Reaction of 3-Diazoindolin-2-imines with 1,3-Dienes in One-Pot

Dahee Park, Gi Hoon Ko, Yongjoo Yun, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

N-Containing heterocyclic compounds are extremely important in the study for biological activity and pharmaceutical utilization. Especially, azepinoindoles having both indole and azepine moieties, which are one of the most typical privileged scaffolds, exhibit antifungal properties and function as antilipase, kinase inhibitor, and H1-receptor antagonist. Herein, we developed rhodium-catalyzed formal aza-[4 + 3] cycloaddition reaction of 3-diazoindolin-2-imines with 1,3- dienes for the synthesis of azepinoindoles in good to excellent yields in one-pot. First, rhodium-catalyzed [2 + 1] cycloaddition reaction smoothly took place to produce iminyl vinyl cyclopropane intermediate at room temperature in chlorobenzene for 1 h, which was thermally converted to azepinoindoles through aza-Cope rearrangement.



Poster Presentation : **ORGN.P-55**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and photophysical properties of benzothiazole-based fluorescence receptor for detecting Cu(II)

Wonsik Na

chemistry, Yonsei University, Korea

Development of chemosensor for recognizing metal cations is important, because heavy metal can adversely affect the human immune system and environmental pollution. Chemosensors that recognize metal cation were developed in this project. To effectively perceive a metal cation, tosyl functional group were introduced as a binding site. Tosyl group can be a binding subunit having great affinity with metal cation. Benzothiazole was added as a binding and signaling subunit. The chemosensor is capable of estimating Cu(II) with a wide concentration range without the interference from other metal ions.

Poster Presentation : **ORGN.P-56**

Organic Chemistry

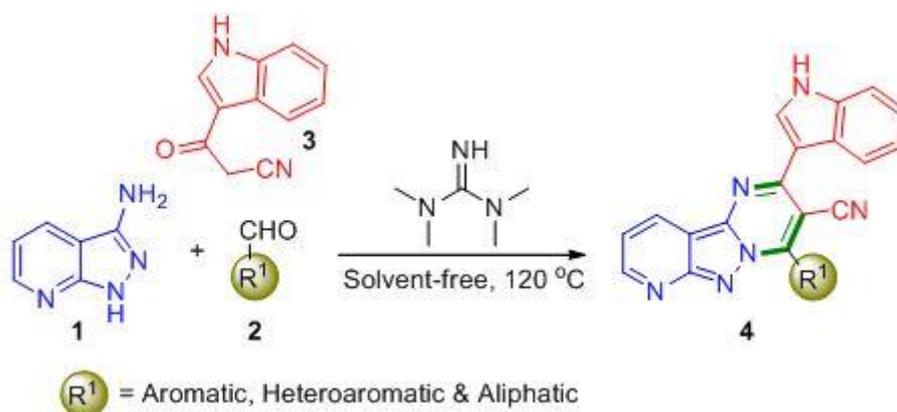
Grand Ballroom, THU 11:00~12:30

An efficient and solvent-free one-pot multi-component synthesis of novel highly substituted pyrido[2',3':3,4]pyrazolo[1,5-a]pyrimidine-3-carbonitrile derivatives catalyzed by tetramethylguanidine

Yeon Tae Jeong*, Kumar Krishnamma

Department of Display Engineering, Pukyong National University, Korea

An efficient solvent-free access towards highly substituted pyrido[2',3':3,4]pyrazolo[1,5-a]pyrimidine-3-carbonitrile derivatives has been established through multi-component reaction of 1H-pyrazolo[3,4-b]pyridin-3-amine, aldehyde, 3-(1H-indol-3-yl)-3-oxopropanenitrile catalyzed by 1,1,3,3-tetramethylguanidine (TMG). The reaction allows the formation of one C–C and two C–N bonds with high yield. The significant features of this solvent-free reaction include mild reaction condition, readily accessible substrates, short reaction time, excellent yield, and broad substrate scopes as well as simple one-pot operation, no column chromatographic purification, which makes this strategy highly attractive.



Poster Presentation : **ORGN.P-57**

Organic Chemistry

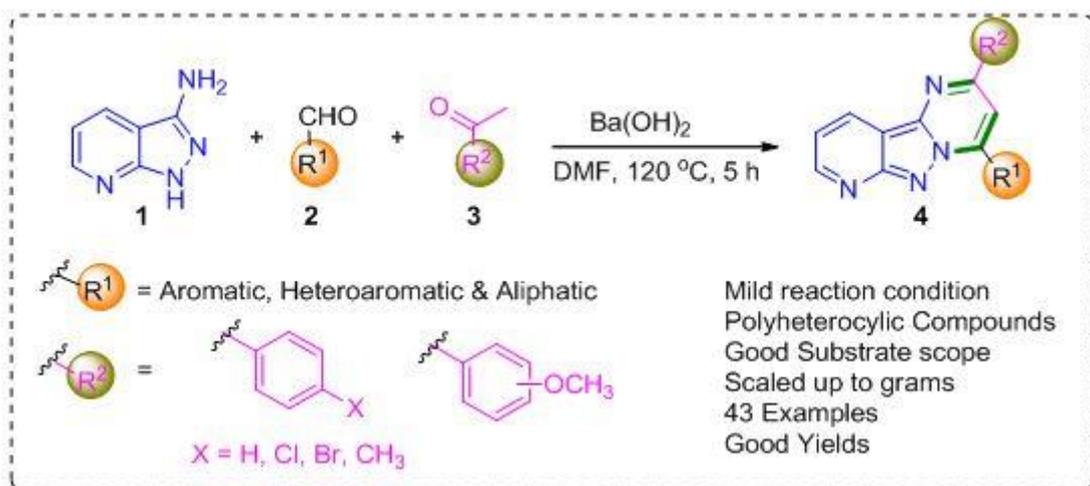
Grand Ballroom, THU 11:00~12:30

An efficient and transition metal-free base-promoted multi-component synthesis of aza-fused polysubstituted pyrido[2',3':3,4]pyrazolo[1,5-a]pyrimidine derivatives

Yeon Tae Jeong*, Kumar Krishnamma

Department of Display Engineering, Pukyong National University, Korea

An efficient and concise practical protocol for the synthesis of novel aza-fused polysubstituted pyrido[2',3':3,4]pyrazolo[1,5-a]pyrimidine derivatives from a readily available aromatic aldehyde, acetophenone and 1H-Pyrazolo[3,4-b]pyridin-3-amine in presence of Ba(OH)₂, under transition metal-free conditions, has been established. This transformation presumably occurs through a sequential Aldol reaction, imine-formation, intramolecular N-cyclization, auto-oxidation sequence of reactions. This protocol, which includes the formation of new C–C and C–N bonds, features a wide substrate scope with a broad range of functional group tolerance.



Poster Presentation : **ORGN.P-58**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

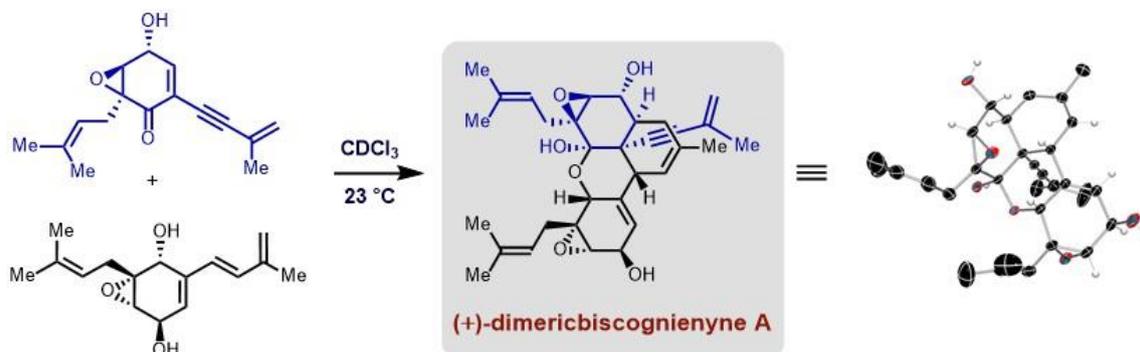
(+)-Dimericbiscognienyne A: Total Synthesis and Mechanistic Investigations of the Key Heterodimerization

Geon Kim, Hee-yoon Lee^{1,*}, Sunkyu Han^{1,*}

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

The first total synthesis of (+)-dimericbiscognienyne A1 is described. Key to the successful access to (+)-dimericbiscognienyne A was the biosynthetically inspired Diels–Alder reaction between two differential epoxyquinoid monomers and the subsequent intramolecular hemiacetal formation. The selective formation of the natural product among other potential diastereomers during the late stage [4+2] cycloaddition reaction was investigated by DFT calculations and experimental control studies.



Poster Presentation : **ORGN.P-59**

Organic Chemistry

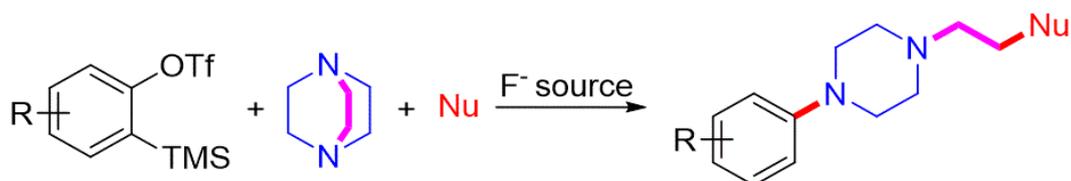
Grand Ballroom, THU 11:00~12:30

Three-Component Reactions of Arynes, Amines, and Nucleophiles via a One-Pot Process

Jeongseob Seo, Haye Min Ko*

Department of Bio-nanochemistry, Wonkwang University, Korea

An unprecedented three-component reaction of arynes, tertiary amines, and nucleophiles has been demonstrated through ammonium salt intermediates. This protocol allows access to tertiary aniline derivatives containing the piperazine motif in good-to-excellent yields. Expansively, this reaction can produce biologically important 2-(4-phenylpiperazin-1-yl)ethyl-containing molecules using arynes, 1,4-diazabicyclo(2.2.2)octane (DABCO), and nucleophiles via a one-pot process.



- Transition-metal free
- C-N bond cleavage and C-Nu bond formation

Poster Presentation : **ORGN.P-60**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Design and synthesis of CNT-Chitosan-Ni and CNT-Chitosan-Pd nanohybrid catalytic platform and its application to the ipso-hydroxylation of arylboronic acids

Minji Kim, Eunjae Shin¹, Seongryu Joo², Seung-Hoi Kim^{2,*}

Dankook University, Korea

¹*Chemistry, Dankook University, Korea*

²*Department of Chemistry, Dankook University, Korea*

we have developed an efficient, economical, and practical strategy for the synthesis of functionalized phenols via the ipso-hydroxylation of arylboronic acids using recyclable, reusable Pd- or Ni-catalyst platform under mild conditions. The developed method has the following advantages such as cost-effectiveness using a versatile oxidant (H₂O₂), and, more importantly, recyclability of the catalyst. Additionally, the easy workup procedure that yields pure products is highly beneficial. Overall, we believe that this approach is the first example of the use of a palladium- or nickel-catalyst in the ipso-hydroxylation of arylboronic acids.

Poster Presentation : **ORGN.P-61**

Organic Chemistry

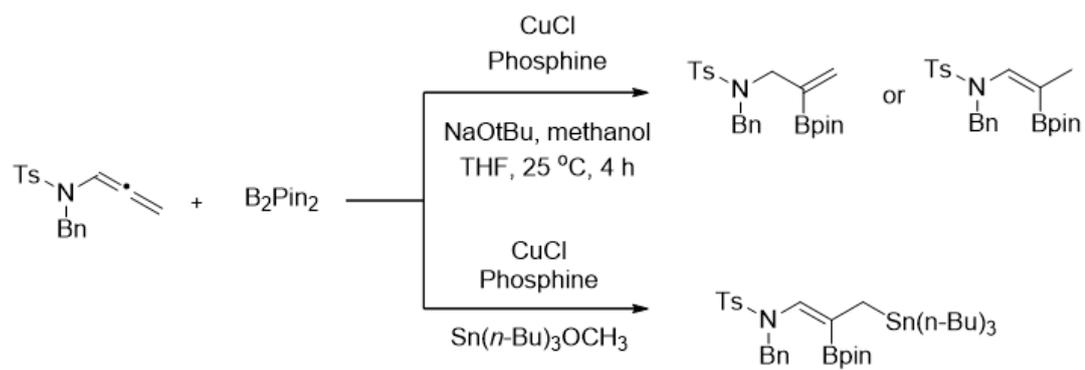
Grand Ballroom, THU 11:00~12:30

Ligand-Controlled Copper-Catalyzed Regioselective Hydroborylation and Borylstannylation of Allensulfonamides

Haeun Lee, Jin Kyoong Park*

Department of Chemistry, Pusan National University, Korea

Bimetallic alkenes have been proven to be versatile compounds for the formation of multi-functionalized valuable compounds through carbon-carbon and carbon-hetero atom bond formations by wisely choosing the coupling partners. Therefore, the transformation of bimetallic species that allow the introduction of diverse functionalities will be a highly demandable owing to the differential reactivities associated with them. In a careful consideration of these features and continuation of our recent research on temporary coordination of a neighboring sulfone group to a metal for stereoselectivity control, herein, we are presenting the results of a highly regio- and stereoselective copper-catalyzed hydroborylation of allensulfonamide with bis(pinacolato)diboron. The subsequent trapping of the intermediate by tri-n-butyltinmethoxide allowed a three-component coupling with same reactivity. Because of the equilibrium associated with this type of functionalized stannane alkenes, however, we observed the formation of only linear β -borylated allyltin under the same reaction condition. We also demonstrated the diverse transformations using these bimetallics compound to many interesting compounds. Reference 1. S. B. Thorpe, X. Guo, W. L. Stantos, *Chem. Commun.* 2011, 47, 424; b) B. Jung, A. H. Hoveyda, *J. Am. Chem. Soc.* 2012, 134, 14902. W. Yuan, S. Ma, *Adv. Synth. Catal.* 2012, 354, 1867; d) F. Meng, B. Jung, F. Haeffner, A. H. Hoveyda, *Org. Lett.* 2013, 15, 14143. Yuki akemoto, Hiroto Yoshida, Ken Takaki, *Synthesis* 2014, 46, 3024–3032



Poster Presentation : **ORGN.P-62**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Oxazolylamines through Copper-catalyzed Electrophilic Amination with Organomagnesium Reagents

Sangback Lee, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

Heteroaryl amines are prevalent compounds found in numerous pharmacologically active compounds and natural products. The classical approaches for the synthesis of heteroaryl amines involve Buchwald-Hartwig aminations, Ullmann-Goldberg coupling reactions, and transition-metal catalyzed oxidative coupling reactions using nucleophilic amines. Copper-catalyzed electrophilic amination using O-benzoylhydroxylamines as electrophilic amine sources can be an alternative route for forming C-N bonds. In this methodology, various organometallic reagents (e.g. organozincs, -magnesiums, -borons and -silicons) have been used as nucleophilic sources. In our study, we developed Cu-catalyzed one-pot electrophilic amination reaction of O-benzoylhydroxylamines with readily prepared heteroarylmagnesium reagents, which were generated in situ from the magnesiation of oxazole derivatives with isopropylmagnesium chloride. The catalytic reaction in the presence of Cu(OAc)₂ and ZnCl₂ effectively provided a variety of oxazolylamine products with high yields.

Poster Presentation : **ORGN.P-63**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

One-Pot Synthesis of 3-Substituted-2-Quinolone derivatives

Byunghoon Ahn, Ill young Lee¹, Hee Nam Lim^{1,*}

Department of Chemistry, Korea University, Korea

¹Eco-Friendly New Materials Research Center, Korea Research Institute of Chemical Technology, Korea

Herein, we describe a copper-mediated practical synthesis of 3-amido-2-quinolones in a one-pot reaction with 2-bromoarylaldehydes and malonamides. The morphologically distinct dendritic copper powder is discovered to promote condensation and the C-N bond formation. This method is complementary to conventional approaches using the Friedländer type reaction. It is economic due to use of inexpensive copper powder, and user friendly by easy setting.

Poster Presentation : **ORGN.P-64**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Pd-Catalyzed Regio- and Stereoselective Synthesis of (*E*)-3-Arylmethyleneisindolin-1-ones

TaeYun Ko, So Won Youn*

Department of Chemistry, Hanyang University, Korea

3-Arylmethyleneisindolin-1-ones are known to exhibit various biological activities and have been utilized for the synthesis of numerous natural products and pharmacologically important compounds. Recently, we developed a Pd-catalyzed one-pot synthetic method of (*E*)-3-arylmethyleneisindolin-1-ones from *N*-Ts-benzamides and styrenes with high regio- and stereoselectivities. In addition, this method could be used as a key step in the total syntheses of aristolactam BII and FI, which are the shortest ones to date.

Poster Presentation : **ORGN.P-65**

Organic Chemistry

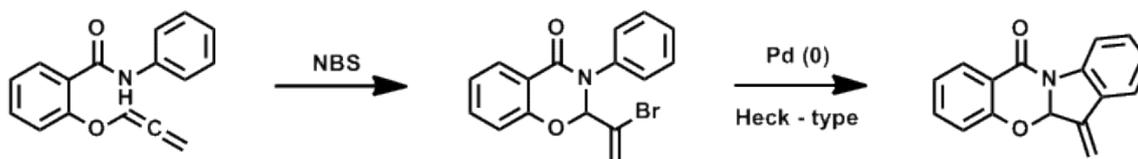
Grand Ballroom, THU 11:00~12:30

Synthesis of dihydrobenzoxazinone derivatives having conjugated substituents from benzamide-aminoallenylethers

Yeonji Kim, Gyeongmin Lee, Sangmin Lim, Guncheol Kim*

Department of Chemistry, Chungnam National University, Korea

A benzamide-aminoallenylether compound was made from salicylic acid in three steps to synthesize the heterocyclic ring of the benzoxazine derivative. The haloamidation proceeds using NBS to perform the cyclization reaction. After synthesis of vinyl halide compounds, the next reactions with Pd(0) catalyst have been tried to prepare dihydrobenzoxazinone derivatives.



Poster Presentation : **ORGN.P-66**

Organic Chemistry

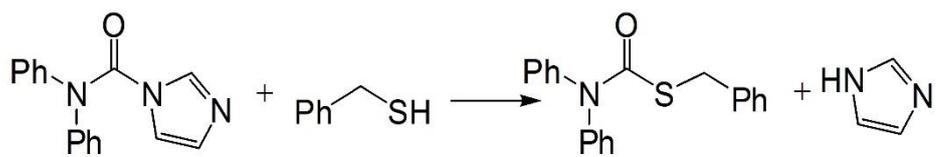
Grand Ballroom, THU 11:00~12:30

Imidazole Derivatives as Thermal Latent Curing Agents for Thiol-Michael Reaction Thermosetting Resins

Sang Hee Lee^{*}, Ghellyn Gajeles, Dong Hee Kim

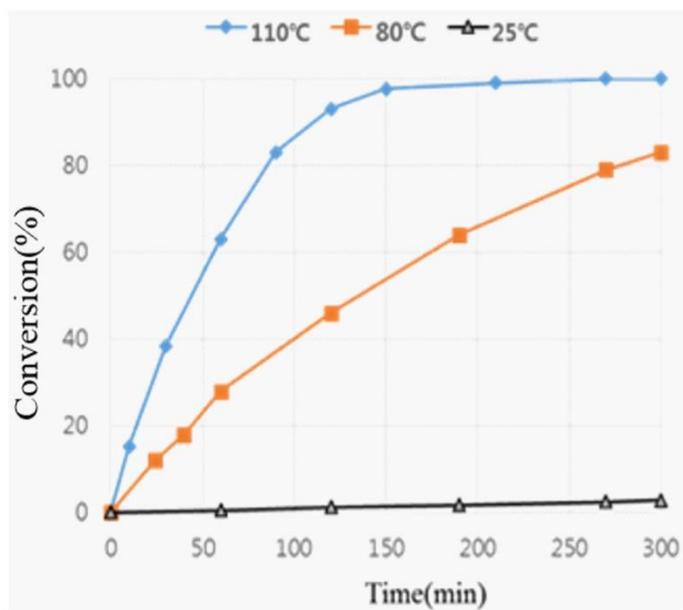
Department of Chemistry, Kunsan National University, Korea

Sulfone containing polymer have high Abbe's number and high refractive index. In the polymerization reaction of thiol and vinyl sulfone, imidazole act as a nucleophilic catalyst. However, unmodified imidazole can cure at room temperature, requiring lower temperature storage of resin formulations to prolong their pot-life. In this study, electron withdrawing group such as carbonyl group introduced to imidazole to decrease nucleophilicity of imidazole. Carbonylated imidazole is inert toward to vinyl sulfone group. Therefore, the viscosity of the monomer mixture can be controlled, giving enough time for homogenizing and degassing procedure. Imidazole derivatives should readily release active imidazole catalyst at a high temperature when attached with a thiol monomer. In model study, modified imidazoles were evaluated by reaction with benzyl mercaptan and applied to polymerization of polythiol and divinyl sulfone.



7 (non-nucleophilic)

Imidazole(nucleophilic)



Poster Presentation : **ORGN.P-67**

Organic Chemistry

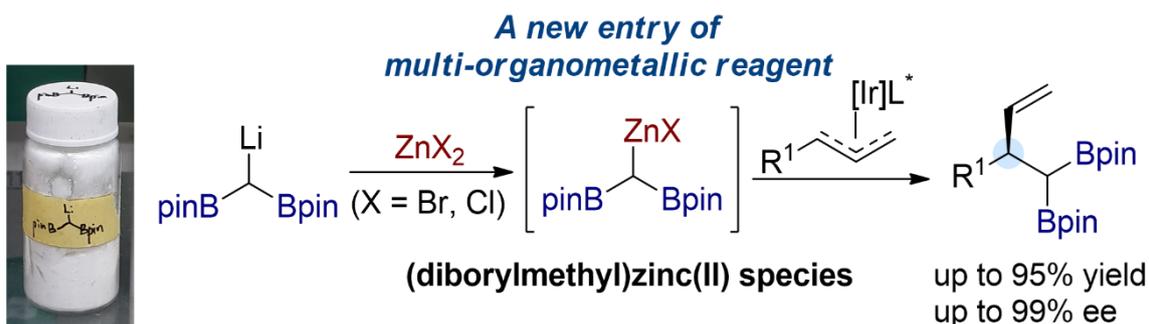
Grand Ballroom, THU 11:00~12:30

Generation and Application of (Diborylmethyl)zinc(II) Species: Access to Enantioenriched *gem*-Diborylalkanes by an Asymmetric Allylic Substitution

Yeosan Lee, Jinyoung Park, Seung Hwan Cho*

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

We report the successful generation of (diborylmethyl)zinc(II) species by transmetalation between isolable (diborylmethyl)lithium and zinc(II) halide (X = Br, Cl) and their application in the synthesis of enantioenriched *gem*-diborylalkanes bearing a stereogenic center at the β -position of the diboryl groups by an asymmetric allylic substitution reaction. The reaction has a broad substrate scope, and various enantioenriched *gem*-diborylalkanes can be obtained in good yields with excellent enantioselectivity. Further elaboration of the enantioenriched *gem*-diborylalkanes provides access to a diverse set of valuable chiral building blocks.



Poster Presentation : **ORGN.P-68**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Combination of Ir(III) Complex and Cancer-Environment-Customized Nanogel for Efficient Photodynamic Therapy

Chae Gyu Lee, Byeong-Su Kim^{1,*}, Tae-Hyuk Kwon*

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

¹Department of Chemistry, Yonsei University, Korea

Ir(III) complexes have attracted much attentions in bio-imaging and targeted therapies due to their outstanding advantages such as large Stokes shift, short incubation time, long luminescence lifetime, enhanced photo-stability and simple color tuning method. Furthermore, Ir(III) complexes showed remarkable efficiency of reactive oxygen species (ROS) generation as photosensitizers via electron (type I) and energy transfer (type II). Despite these great characteristics, the use of Ir(III) complexes as therapeutic agents has been limited because of their poor biocompatibility and water solubility.

Herein, we provide reduction-triggered self-cross-linked nanogel which is compatible with iridium complexes and hydrophilic. We synthesized iridium complexes(**TIr3**) encapsulated in self-cross-linked hyperbranched polyglycerol nanogels(Naph-P(G-co-SSG) nanogels) by using the thiol-disulfide intermolecular exchanges. This Ir(III) complex involved nanogel was much soluble in physiological environments compared to the Ir(III) complex. Through DLS and TEM, the size of nanogels were confirmed and release profile of iridium complex in physiological environment were detected by UV-vis absorption. With these formed nanoparticles, we expect enhancement of cell viability and photo-toxicity index for cancer cells due to better biocompatibility and enhanced permeability and retention (EPR) effect of nanoparticles.

Poster Presentation : **ORGN.P-69**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

[Withdrawal] Facile Synthesis of A New Family of BODIPY Analogues

Khyarul Alam, Jae Won Kim, Jin Kyoong Park*

Department of Chemistry, Pusan National University, Korea

- Withdrawal -

Poster Presentation : **ORGN.P-70**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

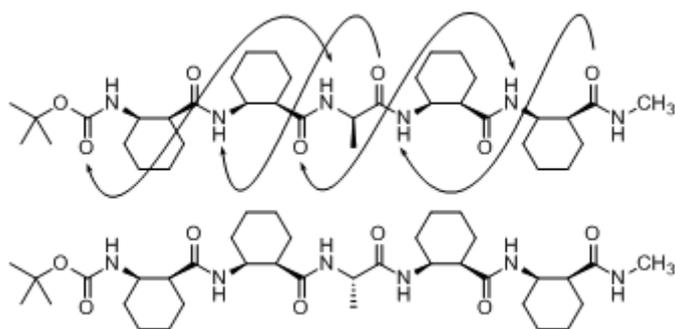
Folding structure owing to introduction of an α -amino acid into the *cis*-2-aminocyclohexanecarboxylic acid oligopeptide

Seung Chan Yoo, Younghun Kim¹, moon-gun Choi¹, Soo Hyuk Choi^{1,*}

Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

The *cis*-2-aminocyclohexanecarboxylic acid (*cis*-ACHC) oligopeptides with alternating chirality have been known to display both right- and left-handed 12/10-helical conformations in solution. We synthesized several *cis*-ACHC pentapeptides of which the third residue is substituted with a simple α -amino acid such as alanine, valine, and 2-aminoisobutyric acid (Aib). Then, we analyzed how introduction of the α -amino acid into the *cis*-ACHC pentapeptide can alter its folding structure by using the CD, 2D-NMR and the single-crystal XRD methods. Herein we demonstrate that introduction of D-alanine or D-valine can promote an intramolecular hydrogen bond to form a left-handed helical structure in this *cis*-ACHC pentapeptide. In contrast, introduction of L-alanine or Aib can interfere helical folding.



Poster Presentation : **ORGN.P-71**

Organic Chemistry

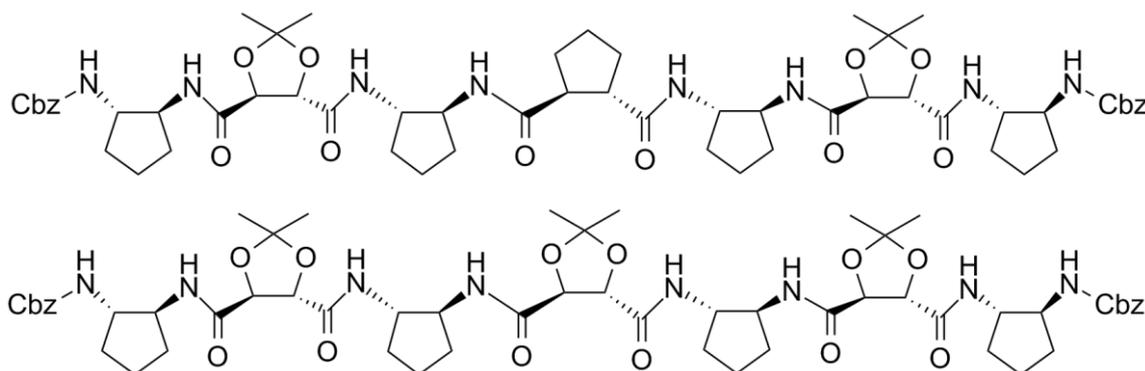
Grand Ballroom, THU 11:00~12:30

Unusual helical structure nylon-like oligomers containing cyclic dicarboxylic acid and diamine residues

Sunglim Choi, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

In the previous study, we synthesized and studied various oligomers using cyclic β -amino acids such as amino cyclopentane carboxylic acid (ACPC) and amino cyclohexane carboxylic acid (ACHC). In particular, trans compounds form beta sheets, showing that they form 10/12 or 12/10 helix structures using cis compound. In this study, we tried to implement helical structures of nylon-like oligomers, which were synthesized using 1,2-diamine and 1,2-dicarboxylic acid. However, synthesized oligomers with acyclic residues were not robust, so cyclic residues were incorporated into oligomers, because we expected that helical propensity of the oligomers is enhanced. In addition, cyclic residues may increase the solubility in organic solvents. For the above reasons, the oligomers were synthesized using acetoneide and cyclopentane diamine. And we analyzed synthesized compounds through CD, IR, and 2D NMR.



Poster Presentation : **ORGN.P-72**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Practical and Efficient Strategy for Synthesis of Aromatic Abietane Diterpenoids from Geraniol

Young Seok Kim, Taejung Kim¹, Sinae Lee², Joonseong Hur¹, Euna Ko³, WonJo Jeong, Yurngdong Jahng^{4,*}, Jae Gyu Park^{5,*}, Jungyeob Ham^{1,*}

Gangneung-Wonju National University, Korea

¹*Natural Products Research, Korea Institute of Science and Technology, Korea*

²*Department of Chemistry, Korea Institute of Science and Technology, Korea*

³*Chemistry, Gangneung-Wonju National University, Korea*

⁴*Yeungnam University, Korea*

⁵*# Advanced Bio Convergence Center (ABCC), Pohang TechnoPark Foundation, Korea*

Aromatic abietane diterpenoids are naturally occurring phenolic tricyclic compounds that have a wide range of biological properties, including antitumor, antimicrobial, antiviral, antiulcer, antileishmanial, antiplasmodial, antifungal, cardiovascular, antioxidant, antibacterial as well as anti-inflammatory activity. Among these compounds, C-12 (and C-7) oxidized aromatic abietane compounds: ferruginol, sugiol, and sugiol methyl ether isolated from *Podocarpus ferrugineus*, *Juniperus communis* L., and *Melia azadirachta* Linn., respectively, have been most widely investigated in the field of natural products synthesis and biological studies. In addition, increased biological activities of these synthetic derivatives possessing an aromatic C-ring have been reported. Thus, the unique and simple structure of aromatic abietane diterpenoids can be used as a template for lead compounds in the development of new drugs that are derived from natural products. Although several methods have been developed for the synthesis of aromatic abietane diterpenoids, some have disadvantages including multiple steps, tedious separation, and expensive starting materials. Herein, we report a practical and efficient strategy for the synthesis of three aromatic abietane diterpenoids from a simple starting material: geraniol. In this poster, detailed synthetic routes will be described.

Poster Presentation : **ORGN.P-73**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Characterization of BTBT Derivatives as Solution-Processable Organic Semiconductors for Organic Thin-Film Transistors

Min-Hwi Son, Sungyong Seo^{1,*}

Pukyong National University, Korea

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

Novel thiophene[1]benzothieno[3,2-b]benzo-thiophene (BTBT) derivatives were synthesized and characterized as solution-processable organic semiconductors for top-contact/bottom-gate organic field-effect transistors (OFETs). Physicochemical properties of the new compounds were characterized by UV-Vis absorption spectroscopy, thermogravimetric analysis (TGA), differential scanning calorimeter (DSC), cyclic voltammetry (CV), and density functional theory (DFT) calculation. The electrical properties of the corresponding compounds were investigated through the fabrication and characterization of field-effect transistors via solution-shearing. Both compounds were FET active and exhibited decent p-channel activity with carrier mobilities up to $0.10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and current on/off ratio $> 10^8$. Film morphology and microstructure, as characterized by atomic force microscopy (AFM) and X-ray diffraction (XRD) were correlated with the device performance.

Poster Presentation : **ORGN.P-74**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Characterization of Benzothiadiazole-based Organic Semiconductors for OTFT and Complementary-like Inverters

YeongKyu Yun, Sungyong Seo^{1,*}

Pukyong National University, Korea

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

New benzothiadiazole derivatives, 4,7-bis(5-phenylthiophen-2-yl)benzo[c][1,2,5]thiadiazole (PT-BTD) and 4,7-bis(4-(thiophen-2-yl)phenyl)benzo[c][1,2,5]thiadiazole (TP-BTD), were synthesized and characterized as small molecular organic semiconductors for organic thin-film transistors (OTFTs) and complementary inverters. Thermal, optical, and electrochemical properties of the new compounds were fully characterized. For the fabrication of thin films based on new compounds, vacuum deposition and solution-shearing method were employed. Thin films based on PT-BTD exhibited p-channel characteristics with hole mobility as high as $0.10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and current on/off ratio $> 10^7$ for top-contact/bottom-gate OTFT devices. With an optimized blending ratio of PT-BTD and the representative n-channel semiconductor, PDIFCN2, bulk heterojunction (BHJ) ambipolar transistors were fabricated with balanced hole and electron mobility of 0.10 and $0.07 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, respectively. Furthermore, a complementary-like inverter using ambipolar thin-film transistors was fabricated, which showed high voltage gain of 84.

Poster Presentation : **ORGN.P-75**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of New Molecules with D-A- π -A-D Configurations Based on Phenothiazine and Quinoline.

So Dam Kim, Tae Woo Kwon*

Department of Chemistry, Kyungsoong University, Korea

We designed and synthesized new molecules with Donor-Acceptor- π -Acceptor-Donor (D-A- π -A-D) configurations based on phenothiazine and quinoline. Phenothiazine has electron rich atoms such as sulfur and nitrogen. It is potentially better electron donor than others because of its non-planar geometry, good thermal and electrochemical stability. Quinolines are well known to be a good electron acceptor materials and thermally stable. In this study, we report the synthesis of 2,2'-(6,6'-(9,9-dihexyl-9H-fluorene-2,7-diyl)bis(4-phenyl-3-(p-tolyl)quinoline-6,2-diyl))bis(10-phenyl-10H-phenothiazine) (FTQP, 1) and 2,2'-(6,6'-(9,9-dihexyl-9H-fluorene-2,7-diyl)bis(3,4-diphenylquinoline-6,2-diyl))bis(10-phenyl-10H-phenothiazine) (FQP, 2) via Ullmann, Grignard, Friedlander condensation and Suzuki coupling reactions. Products were determined by using ¹H, ¹³C NMR, LC-MSMS, UV-Vis, Photoluminescence, TGA and DSC. Detailed synthetic routes and characterization of materials will be described.

Poster Presentation : **ORGN.P-76**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Studies on the Diastereoselective Synthesis of Phosphorodiamidate Morpholino Dimers

Sojeong Min, Keun ho Chun *

Chemistry, Soongsil University, Korea

Phosphorodiamidate morpholino oligonucleotides (PMO) are one of the antisense artificial genes that can bind natural DNA or RNA. PMO is a noncharged nucleotide analogue that can hybridize complementary DNA or RNA with higher affinity and specificity than unmodified DNA–DNA and DNA–RNA duplexes. However, there is a disadvantage that stereoisomers are formed in phosphate during polymer formation. Studies on the control of stereochemistry using metal catalysts in the synthesis of morpholino nucleoside have been published, but no studies on the stereoselectivity in the polymer formation process including dimer have been published yet. In this study, we tried to control the stereoselectivity in the formation of PMO dimers by using various Lewis acid catalysts. So far, LiBr or 9-BBN showed relatively good results. In addition to the catalyst, the nature of the protecting groups attached to the OH and NH groups of the morpholino nucleoside has also been found to have a significant effect.

Poster Presentation : **ORGN.P-77**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Mitochondria-targeting peptoids

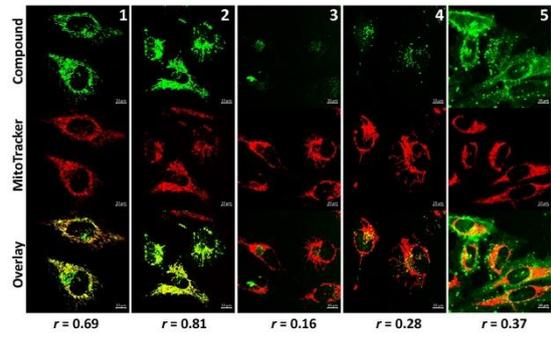
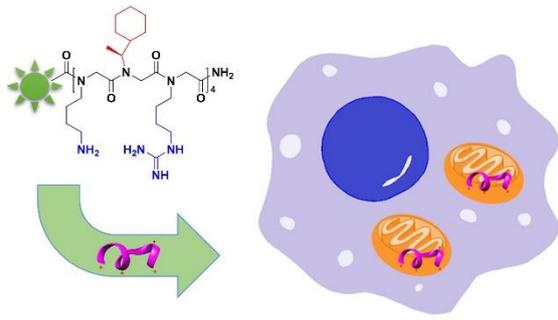
Ho Yeon Nam, Jiwon Seo^{1,*}, Jiyoun Lee^{2,*}

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

¹*Gwangju Institute of Science and Technology, Korea*

²*Global Medical Science, Sungshin University, Korea*

Mitochondria are known to be involved in cellular metabolism, calcium homeostasis, and signal transduction. Accumulated damage caused by singlet oxygen, from performing the various roles, provokes mitochondrial dysfunction. In particular, various diseases such as cancer, diabetes, and neurodegenerative disorders have been reported to be associated with damage to mitochondria. Therefore, mitochondria-targeting vehicles have been actively studied as therapeutic methods for the removal or recovery of damaged mitochondria. Small molecules and peptide-based compounds have been reported, but cargo-dependent toxicity or proteolytic degradation reduces the efficiency of a specific mitochondria-targeting transporter. To circumvent this, we developed a new kind of mitochondria-targeting method. Peptoids are N-substituted oligoglycines and have been selected as promising candidates to complement existing methods. Guanidine-rich and hydrophobic sequences are known to be essential for targeting mitochondria, and various types of hydrophobic monomers have been introduced to test their efficiency. Among them, the peptoid containing the cyclohexyl monomer showed the highest effect on cellular uptake and mitochondrial localization, and its toxicity was also found to be very low. In addition, compounds with secondary structures exhibited better activities than those without, showing a relationship between structure and biological activity. The present mitochondria-targeting peptoids are expected to be able to selectively deliver various biologically active species to minimize side effects in future mitochondrial-related disease treatment studies.



Poster Presentation : **ORGN.P-78**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Fluorescent Ion Pair Receptor for Selective Recognition of Lithium Chloride

Juho Yang, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Fluorescent ion pair receptors were designed and synthesized for selective recognition of LiCl. They consist of tripodal pyridine units for cation recognition and urea groups linked to the pyridine groups as anion binding motifs. The pyrene was also introduced into the receptors as a fluorescent signaling unit. ¹H NMR and fluorescence spectroscopic analysis revealed that the receptors possessed an ability to bind LiCl with high selectivity over other chloride salts. Upon exposure of the receptor to LiCl, significant fluorescence enhancement was observed as a result of LiCl binding with the receptors inhibiting PET (photo-induced electron transfer).

Poster Presentation : **ORGN.P-79**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Calix[4]pyrrole Biscrowns Having a Deep Cavity and Their Ion Pair Recognition

Hye Jin Han, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

New ion pair receptors having deep cavities were prepared based on calix[4]pyrroles doubly strapped with crown ethers having various ring sizes. It was revealed by ^1H NMR spectroscopic analysis that the receptors were able to bind CsF highly selectively over other alkali metal halide salts. In this case, the cesium cation was bound to the crown ether moieties with the fluoride anion being hydrogen bonded to the calix[4]pyrrole NHs. ^1H NMR spectroscopic analysis also provided an evidence that the calix[4]pyrrole biscrowns form complexes with a specific cation such as the sodium in the absence of anions bound to calix[4]pyrroles.

Poster Presentation : **ORGN.P-80**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of a crown ether strapped calix[4]pyrrole and its ion pair recognition

Nam Jung Heo, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new ion pair receptor based on calix[4]pyrrole strapped with a bisazacrown ether was synthesized. This receptor consists of calix[4]pyrrole having two phenoxy walls and a diaza crown ether linking diagonal phenoxy groups. The ion pair receptor was found to be able to bind various ion pairs such as alkali metal halide salts. In this case, the metal cation was complexed to the bisazacrown ether ring whereas the anions were bound to the calix[4]pyrrole. More details on ion pair binding properties of the ion pair receptor will be presented.

Poster Presentation : **ORGN.P-81**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Phenanthroline Strapped Calix[4]pyrroles with High Selectivity for the Bicarbonate Anion

JeongHyeon Kim, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Phenanthroline strapped calix[4]pyrroles with ester and amide linkages were synthesized. ^1H NMR spectroscopic analyses revealed that the calix[4]pyrrole having the ester linkages is capable of binding LiCl with high selectivity over other alkali metal chloride salts. In this case, the lithium cation was complexed with the phenanthroline moiety while the chloride anion was hydrogen bonded the pyrrolic NHs of the calix[4]pyrrole unit. By contrast, the strapped calix[4]pyrrole with the amide linkages was found to bind the bicarbonate anion with significantly high affinity and selectivity.

Poster Presentation : **ORGN.P-82**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Oxoanion Recognition by a Molecular Cage

Juhyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A 3-dimensional cage molecule **1** was synthesized by following multistep synthetic procedure. Cage **1** contains both hydrogen bonding donors such as amides and pyrroles and hydrogen bonding acceptors such as imines. ^1H NMR spectral titrations showed that cage **1** binds oxoanions such as the dihydrogen phosphate, the hydrogen sulfate, and the sulfate anion via slow binding/release equilibriums on the ^1H NMR time scale. These findings led us to conclude that cage **1** has an ability to bind such oxoanions with relatively high affinity as compared to other anions including halide anions. The 1:1 binding stoichiometry between the receptor and the anions were proved by Job's plot experiments. Single crystal X-ray diffraction analysis provided further evidence that receptor **1** forms a 1:1 complex with the dihydrogen phosphate via multiple hydrogen bonds.

Poster Presentation : **ORGN.P-83**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Heterotritopic Ion Pair Receptor Based on Calix[4]pyrroles and a Bisazacrown Ether

Han-byeol Choi, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new heterotritopic ion pair receptor was synthesized. The receptor was comprised of two calix[4]pyrrole units as an anion binding motif and the bisazacrown-6 for cation recognition. ¹H NMR spectroscopic analysis revealed that the crown ether moiety forms strong intramolecular hydrogen bonds with the calix[4]pyrroles inhibiting the ability of the calix[4]pyrroles to bind anions. On the contrary, when the receptor was exposed to the calcium cation, the cation was bound to the bisazacrown ether destroying the intramolecular hydrogen bonds between the crown ether and calix[4]pyrroles. As a result, the calix[4]pyrrole units recovered their anion binding ability eventually to form ion pair complexes with CaX₂.

Poster Presentation : **ORGN.P-84**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Potassium and Cesium Salt Recognition by a Calix[4]crown-5 Strapped Calix[4]pyrrole Multitopic Ion Pair Receptor

Seung Hyeon Kim, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A calix[4]crown-5 strapped calix[4]pyrrole was synthesized as a multitopic ion pair receptor. In this case, the calix[4]arene subunits was locked in the 1,3-alternate conformation whereas the calix[4]pyrrole constituent is conformationally flexible. The ion pair receptor was found to have ability to bind specific ion pairs such as potassium and cesium salts with high selectivity. It was proved by ¹H NMR spectroscopic analyses that the ion pair receptor formed ion complexes with cesium salts and potassium salts via two different binding mods. For example, it formed the cesium salt complexes in which the cesium cation was bound to the crown-5 ring with the anions hydrogen bonded to the calix[4]pyrrole. By contrast, in the cases of potassium salts, the potassium cation was encapsulated in the crown-5 unit with anions located outside the ion pair receptor.

Poster Presentation : **ORGN.P-85**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Designing Transition Metal Catalysts: Ir catalyzed Transfer Hydrogenation Using Glycerol as Sustainable Hydrogen Source

Yeon Joo Cheong, Hye-Young Jang^{1,*}

Department of Energy System, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Transfer hydrogenation is a method that transferring hydrogen atoms to organic compounds in the absence of H₂ gas. Because hydrogen gas used in the reduction process is difficult to handle and dangerous, we investigated a hydrogen source produced by the dehydrogenation reaction of glycerol. Recent interests regarding the utilization of glycerol as a sustainable chemical resource have been increasing. Glycerol is the byproduct of biofuel processes, and the development of the chemical transformation of glycerol would provide benefits in chemical industries. Glycerol also has many chemical advantages. For example, it is non-flammable, non-toxic, and high boiling point property rather than other alcohols such as MeOH and EtOH. It can dissolve inorganic salt, acid, base, metal complex, and organic compounds. In this study, we use glycerol as a reductant for transfer hydrogenation, where various organic compounds including carbonates derived from CO₂ are converted to reduced compounds, and glycerol also is converted to useful chemicals such as lactic acid. So we aimed the reduction of organic compounds using glycerol as a sustainable hydrogen source in the presence of iridium catalysts. Through a preliminary experiment and a plausible mechanism study, we found out that the ligand structure of the catalyst affects the activity. Based on a known Iridium catalyst, we synthesized new iridium catalysts which are highly active in both transfer hydrogenation of carbonates and dehydrogenation of glycerol. In this presentation, we are going to present our novel iridium catalysts and performed transfer hydrogenation of carbonate from CO₂ and glycerol. Detailed conditions will be discussed.

Poster Presentation : **ORGN.P-86**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and properties of terminal amino-oxy modified S1P derivatives

Ji hye Park, YeJi Lee, In seok Hong*

Department of Chemistry, Kongju National University, Korea

Biologically active lipids serve as signaling molecules in human and animal diseases. In particular, sphingosine-1-phosphate (S1P) is secreted in the blood for wound healing and is known to act as an immune cell and cancer cell differentiation, survival, and function regulator. Depending on the level of S1P in the blood, the potential for biomarkers to detect specific diseases or cancer cells is emerging. To make an antibody capable of detecting S1P, a derivative that binds S1P efficiently to the antigen-forming protein is required. Therefore, in this study, we report the efficient synthesis of S1P derivatives with terminal amino-oxy functional groups. The possibility of the terminal amino-oxy S1P derivative as an epitope was confirmed by a known ELISA method. The production of antibodies using these derivatives is currently being studied.

Poster Presentation : **ORGN.P-87**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Mechanism of Palladium-Catalyzed C–N Coupling with DBU as a Base

Seoung-Tae Kim, Mu-Hyun Baik*

Chemistry, Korea Advanced Institute of Science and Technology, Korea

In general, the Buchwald-Hartwig amination reaction employs strong, inorganic or insoluble bases to deprotonate less acidic amines albeit these bases expose innate limitations: i) reduce the functional group tolerance, ii) insoluble in a solvent, iii) air sensitive, and iv) can require higher Pd loadings. Recently, the Buchwald group reported a new Pd-catalyzed C–N cross-coupling reaction that can tolerate highly base-sensitive substrates by using organic-base. In this DFT study, the mechanism of Pd-catalyzed C–N cross-coupling reaction with organic-base, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), is explored. This study addresses the reason for the difficulty of using the organic-base and shed light on the importance of ligand bulkiness for the reaction.

Poster Presentation : **ORGN.P-88**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Safer Synthesis of Tetrazoles from Secondary Amines using Trichloroacetonitrile

Su-jin Oh, Yeong-Gweon Lim*

Agency for Defense Development, Korea

Tetrazoles are aromatic heterocyclic compounds with high nitrogen contents and considered as the promising building block of HIEMs(High-performance Insensitive Energetic Materials) due to their high heat of formation, high stability and environmentally friendly property. Tetrazole derivatives can be generally prepared from secondary amines through cyanation using highly toxic and expensive cyanogen bromide. To overcome these shortcomings, we test the safer cyanation method using trichloroacetonitrile. The scope and limitations of this method are discussed.

Poster Presentation : **ORGN.P-89**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Crystal Structure of 2',6'-dicyano-2,3'-bipyridine and Conformational Comparison between Four Independent Molecules

Suk-Hee Moon, Youngjin Kang^{1,*}, Ki-Min Park^{2,*}

Department of Food & Nutrition, Kyungnam College of Information & Technology, Korea

¹*General Science Education, Kangwon National University, Korea*

²*Research Institute of Natural Science, Gyeongsang National University, Korea*

Bipyridine ligand with the C[^]N-chelating modes to transition metal ion such as 2,3'-bipyridine has considered as strong candidate for synthesizing blue phosphorescent heavy transition metal complexes due to their larger triplet energy (T_1) compared with phenylpyridine based C[^]N-chelating ligand. In particular, the triplet energy of fluorine-functionalized 2,3'-bipyridine (T_1 : 2.82 eV) is larger than that of alkoxy-functionalized analogy, 2',6'-dimethoxy-2,3'-bipyridine (T_1 : 2.70). Therefore, the introduction of electron-withdrawing group into C-coordinating pyridine is highly desirable in order to develop blue phosphorescent metal complexes. To design a suitable ligand possessing large triplet energy is still main issue in organic light-emitting diodes (OLEDs) research area because developing blue phosphorescent materials remains as problem to be solved so far. Although there are number of advantages in 2,3'-bipyridine ligand, incorporating the substituents into ligand framework is hardly approachable owing to low selectivity and reactivity of pyridine ring. In addition, the structural examples of bipyridine bearing electron-withdrawing group are very scarce. Herein, for potential application to the development of blue phosphorescent materials, we present about the crystal structure of 2,3'-bipyridine-2',6'-dicyanitrile, which crystallized in the space group $P2_1/c$ with four crystallographically independent molecules (*A*, *B*, *C*, and *D*) in the asymmetric unit. Furthermore, conformational difference between these independent molecules obtained by the *AutoMolFit* routine in PLATON is also discussed.

Poster Presentation : **ORGN.P-90**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Water-sensitive ratiometric fluorescent probe and its application to test strip for water detection with a rapid and reversible response

Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Naphthalimide-decorated fluorinated acetamides **1** and **2** were developed as a water-sensitive ratiometric fluorescent probe. The **1** and **2** exhibited characteristic dual emission with a large Stokes shift in the presence of water, attributed to the increase of intramolecular charge transfer (ICT) of the naphthalimide moiety through the association of the fluorinated acetamide group with water. In particular, the **1** gave rise to a ratiometric change of the dual emission and a visual fluorescent color change according to the water concentration contained in various organic solvents such as ethanol, methanol, and acetonitrile. Moreover, the **1**-impregnated paper strips showed a rapid and easy-to-visualize fluorescent color change for the detection of water in various solvents, as well as the simplicity and reusability.

Poster Presentation : **ORGN.P-91**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Dimerization of AIEgens for selective detection of H₂S over GSH, Cys and Hcy

Min Jung Chang, Chulhun Kang^{1,*}, Min Hee Lee^{2,*}

Department of chemistry, Sookmyung Women's University, Korea

¹*Graduate School of East-West Medical Science, Kyung Hee University, Korea*

²*Department of Chemistry, Sookmyung Women's University, Korea*

We developed a highly selective fluorescent AIEgen (**1**) that can provide a strong fluorescence at 480 nm for H₂S detection based on a dimerization through thiol-disulfide exchange. As far as we know, this is the first report on dimerization of AIEgens for selective detection of H₂S over GSH, Cys, and Hcy. Probe **1** was also highly selective to H₂S over other ROS, metal ions, anions, and various vapors. In addition, **1** readily provided a detectable fluorescence increase to H₂S in the physiological pH range (4-9) with a detection limit (84 nM) compatible with the biological H₂S levels. Furthermore, we presented a probe **1**-coated glass-backed silica gel TLC plate as an AIEgen-based light-up sensor plate for detection of toxic H₂S gas in air.

Poster Presentation : **ORGN.P-92**

Organic Chemistry

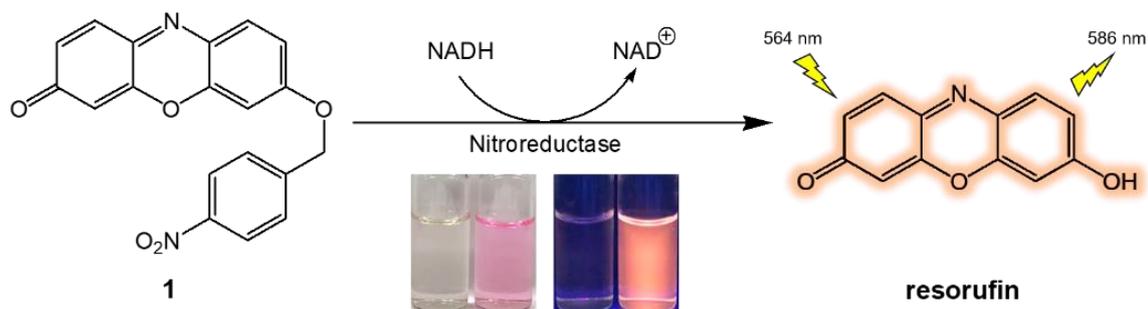
Grand Ballroom, THU 11:00~12:30

A simple resorufin derived fluorescent probe for selective and sensitive detection of nitroreductase in hypoxic tumor

Jung Won Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Increasing biological activity of nitroreductase (NTR) is well-known phenomenon in hypoxic tumors. So, level of NTR is effective measuring method for monitoring hypoxic degree in living systems. More simple, selective, and sensitive probe for detecting NTR is required, and a resorufin derivatives (**1** and **2**) have simple structures and highly selectivity for NTR. The probes give a fluorescent turn-on change at 586 nm with a color change from colorless to pink in the presence of NTR and NADH in aqueous solution. The fluorescent changes of probes were completed in about 20 minutes and turnover numbers of **1** and **2** were $0.260 \mu\text{M}^{-1} \text{s}^{-1}$ and $4.368 \mu\text{M}^{-1} \text{s}^{-1}$, respectively. And we checked **1** is more selective and stable than **2**, through the selectivity test and pH test. Because the efficiency of **1** is much better than **2**, we are studding the bioimaging experiments using **1** are ongoing.



Poster Presentation : **ORGN.P-93**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A mitochondrial NAD(P)H selective fluorescent Off-On probe

Jinhui Joo, Sun Young Park¹, Min Hee Lee^{1,*}

Chemistry, Sookmyung Women's University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Reduced nicotinamide adenine dinucleotide (NADH) and its phosphate ester (NADPH) are the factors involving in many redox reactions in living cells. In particular, the NAD(P)H plays a crucial role in the production of energy in the mitochondria by giving its electron. When NAD(P)H is defective, it causes degenerative diseases such as Parkinsonism and Alzheimer's disease. In this regard, we developed a fluorescent probe **1** for imaging NAD(P)H in the mitochondrial of living cells. This probe consisted of red-emitting fluorophore as the signaling unit as well as NAD(P)H reactive site, and triphenyl phosphonium salt as mitochondria targeting group. The **1** is none-fluorescent, however, upon reacting with NAD(P)H a significant fluorescence increase was monitored in both solution and living MDA-MB-231 cell.

Poster Presentation : **ORGN.P-94**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A hemicyanine-based turn on fluorescent probe for selective detection of glutathione

Jinju Lee, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

We describe a new hemicyanine-based fluorescent probe (**1**) for the selective detection and imaging of glutathione (GSH). Probe **1** was composed of hemicyanine as a fluorophore, trimethyl lock quinone (TLQ) and para-amino benzyl alcohol linker. This probe shows a broad absorption band at 425 nm and a very weak fluorescence intensity around 550 nm. However, upon addition GSH, a significant increase in the fluorescence intensity at 540 nm was observed in the physiological conditions. We confirmed that no fluorescence change was occurred by GSH using various reference compounds. Hence, we assumed that the GSH binding at -NH part of para-amino benzyl alcohol and TLQ group resulting photoinduced electron transfer (PET) off and fluorescence on. The turn-on fluorescent change of **1** is selective for GSH over other anions, metal ions, redox species.

Poster Presentation : **ORGN.P-95**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A coumarin-naphthalimide hybrid as a ratiometric fluorescent probe for hNQO1

Sun Young Park, Chulhun Kang¹, Jongseung Kim², Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

¹*Graduate School of East-West Medical Science, Kyung Hee University, Korea*

²*Department of Chemistry, Korea University, Korea*

Human NAD(P)H:quinone oxidoreductase (hNQO1) promotes a reduction of quinones to hydroquinones in the presence of NADH. It is reported that the hNQO1 activity is higher in cancer cells than in normal cells and it is also associated with a drug resistance factor of cancer cells. Here, we presented a coumarin-naphthalimide hybrid (**1**) containing a trimethyl lockquinone designed as the trigger group as a selective ratiometric fluorescent probe for detecting hNQO1. The trimethyl lockquinone moiety of **1** could be reduced by hNQO1 into hydroquinone which subsequently cyclized, resulting in a production of **2** as well as a ratiometric fluorescence change between 450 and 540 nm. Also, probe **1** was highly selective for hNQO1 activity over other biologically relevant species, including metals, ROS, and anions. In confocal microscopic experiments using the hNQO1-positive A549 cell line, probe **1** displayed a ratiometric fluorescence image through a hNQO1-induced fluorogenic reaction, which was confirmed by the treatment of dicoumarol as a hNQO1 inhibitor.

Poster Presentation : **ORGN.P-96**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Development of Bicyclic Bridgehead Phosphoramidite Ligands for Hydroformylation of Substituted Olefins

Taeil Shin, Kim Hyunwoo*

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

Hydroformylation is one of the powerful tools to make aldehyde using olefins as substrate and carbon monoxide and hydrogen gas in the presence of a metal catalyst. Aldehyde is valuable material for industry filed to make polymer or fragrances. Also, it converted to useful materials such as alcohol or amine via simple reaction.¹ Over the last few decades, many research has been reported on the hydroformylation reaction for mono- or disubstituted alkenes. On the other hand, the hydroformylation of high-substituted olefins such as trisubstituted olefin has not been reported well. Because hydroformylation of trisubstituted olefins requires some specific condition and catalyst. For example, high pressure and temperature require for this reaction and hard to control the selectivity between linear and isomerized aldehyde. Here in, we introduce Rh(I)-catalyzed hydroformylation of substituted olefins by using bicyclic bridgehead phosphoramidite ligands. Our briphos(bicyclic bridgehead phosphoramidite) ligands have an advantage of easily tunable properties such as electronic and steric effect. By using this properties, Briphos ligands show good reactivity and selectivity in hydroformylation of trisubstituted olefins by changing its structures. Modified briphos ligands show much better reactivity and selectivity than other commercial ligands. Among the various briphos ligands, Briphos(t-Bu), which is tert-butyl substituted at ortho and para position of phenyl, shows best reactivity and selectivity for the hydrofmylation of trisubstituted olefins with various substrate.

Poster Presentation : **ORGN.P-97**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Designing Chemoselectivity in Dipolar Cycloadditions : How to Control the Attack Site of Catalyst?

Seung-yeol Baek, Mu-Hyun Baik^{1,*}, Eun Jeong Yoo^{2,*}

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

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

²*Department of Applied Chemistry, Kyung Hee University, Korea*

Cycloadditions are the one of most important chemical reactions in organic chemistry because cyclic products can play a pivotal role in the preparation of natural products, pharmaceutical agents or synthetic materials. Among various cycloaddition reactions, the dipolar cycloadditions provide a desirable route to control the selectivity. In particular, stepwise cycloadditions involving metal-associated reactive intermediates emerged as reliable way of programming selectivity. However, dipolar cycloadditions to afford products that have entirely different skeletons or reaction sites with switchable selectivity remains poorly addressed, although such control should be possible in principle. There is currently no known conceptual strategy for engineering an intrinsic bias for site-control. To identify a rational strategy for programming regioselectivity into dipolar cycloadditions by taking advantage of the intrinsic charge polarization of the substrate, we carried out a combined computational and experimental study. The orbital symmetries of the frontier molecular orbitals were examined and matched by the appropriate transition metal catalyst to gain control over the cyclization mechanism, which in turn gave high levels of regiocontrol.



Poster Presentation : **ORGN.P-98**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Asymmetric Michael Addition of Pyrazolones to Nitroalkene Derivatives Catalyzed by Binaphthyl-modified Squaramide Organocatalyst.

Yonghwan Kim, Dae Young Kim^{1,*}

Soonchunhyang University, Korea

¹*Department of Chemistry, Soonchunhyang University, Korea*

The asymmetric synthesis of pyrazolone derivatives has become the subject of great interest over the past decades. We have developed highly efficient catalytic enantioselective conjugate addition reaction of pyrazol-5-ones to nitroalkenes using binaphthyl-modified squaramide. The desired Michael products were obtained in excellent yields and enantioselectivities (up to 95% ee). We believe that this method provides a practical entry to biologically useful chiral 4-substituted pyrazol derivatives.

Poster Presentation : **ORGN.P-99**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Photocatalytic Difluoromethylation/1,2-Carbon Migration Sequences for the Synthesis of CF₂H-Substituted Cyclopentanones

Yeonjoo Kim, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A visible-light-mediated photocatalytic difluoromethylation /1,2-carbon migration of alkenols is described. This approach provides a mild and operationally simple access to the synthesis of difluoromethyl-substituted cyclopentanones via difluoromethylation and 1,2-carbon migration of 1-(1-arylvinyl)cyclobutanol derivatives.

Poster Presentation : **ORGN.P-100**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Visible light-mediated arylation of quinoxalin-2(1H)-ones with aryldiazonium salts,

Yeonjoo Kim, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A visible light photoredox-catalyzed C-3 arylation of quinoxalin-2(1H)-ones with aryldiazonium tetrafluoroborates has been developed. The reaction was effectively accelerated using an inexpensive eosin Y as a photoredox catalyst under visible-light irradiation without any other metal, oxidant, or additive. This approach offers a facile way to prepare 3-arylquinoxalin-2(1H)-one derivatives with a wide range of functional group tolerance.

Poster Presentation : **ORGN.P-101**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Visible light photoredox-catalyzed arylation of quinoxalin-2(1H)-ones with aryldiazo sulfones under photocatalyst-free condition

Hyeim Jeong, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

We have successfully developed a photocatalyst-free photoredox arylation of quinoxalin-2(1H)-ones with aryldiazo sulfones. The reaction was completed without any other metal, oxidant, or additives. The proposed protocol is a convenient option for the synthesis of 3-arylquinoxalin-2(1H)-one derivatives with a wide range of functional group tolerance.

Poster Presentation : **ORGN.P-102**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Highly enantioselective addition of pyrazolones to ketimines derived from isatins catalyzed by binaphthyl-modified organocatalysts

Hyeim Jeong, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

Chiral binaphthyl-modified squaramide-catalyzed enantioselective addition of pyrazolones to ketimines derived from isatins has been achieved. This method affords practical and efficient access to chiral pyrazolone-substituted oxindole derivatives in high yields with excellent enantioselectivities (up to 99% ee).

Poster Presentation : **ORGN.P-103**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Visible light-mediated photoredox-catalyzed phosphorylation of quinoxalin-2(1H)-ones with phosphine oxide.

Yubin Kim, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A visible light photoredox-catalyzed C-3 phosphorylation of quinoxalin-2(1H)-ones with diphenylphosphine oxide has been developed. The reaction was effectively accelerated using an inexpensive eosin B as a photoredox catalyst under ambient air at room temperature without any other metal, oxidant, or additive. This approach offers a facile way to prepare 3-diphenylphosphorylated quinoxalin-2(1H)-one derivatives.

Poster Presentation : **ORGN.P-104**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Asymmetric synthesis of 2,4-diaryl-1-benzopyrans via organocatalytic asymmetric decarboxylative alkylation of β -keto acids to ortho-quinone methides.

Yubin Kim, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A novel and efficient asymmetric synthesis of 2,4-diaryl-1-benzopyrans via enantioselective decarboxylative alkylation of β -keto acids to o-quinone methide intermediates, followed by sequential cyclization and dehydration has been developed. The synthetically useful chiral 2,4-diaryl-1-benzopyran derivatives were obtained in moderate to high yields and high enantioselectivities through a one-pot, two-step sequence. This approach offers a facile way to prepare chiral 2,4-diaryl-1-benzopyran derivatives with a wide range of functional group tolerance.

Poster Presentation : **ORGN.P-105**

Organic Chemistry

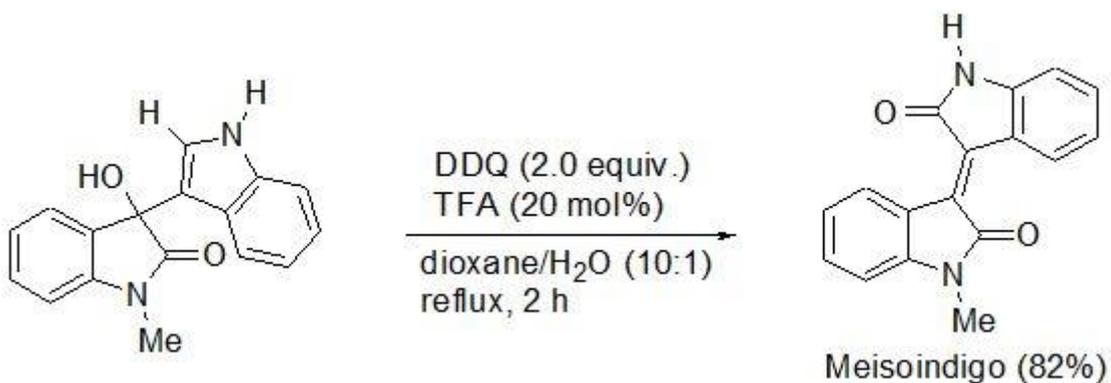
Grand Ballroom, THU 11:00~12:30

Facile Synthesis of Isoindigo Derivatives from 3-Indolyl-2-oxindoles with DDQ

Da Young Seo, Hwa Jung Roh, Jae Nyoung Kim*

Department of Chemistry, Chonnam National University, Korea

Various isoindigo derivatives were synthesized in good yields from 3-indolyl-2-oxindoles by 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) in aqueous 1,4-dioxane in the presence of a catalytic amount of trifluoroacetic acid.



Poster Presentation : **ORGN.P-106**

Organic Chemistry

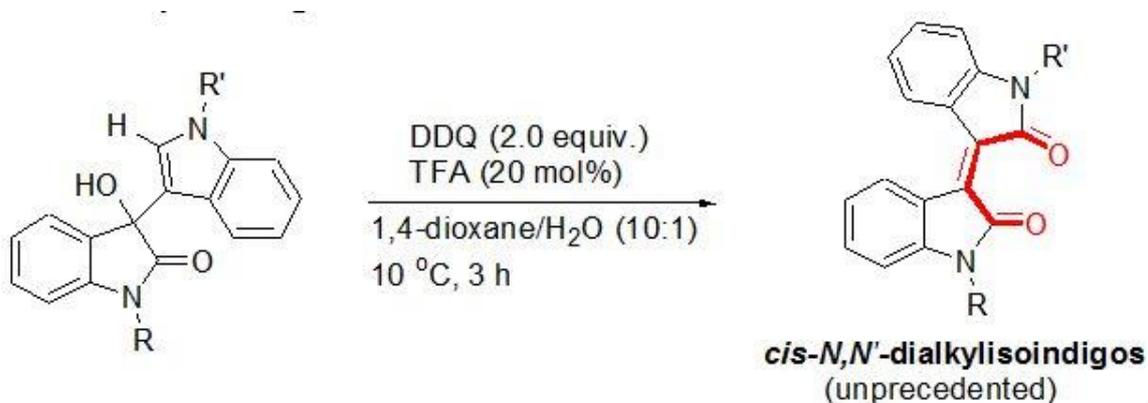
Grand Ballroom, THU 11:00~12:30

The First Synthesis of *cis*-*N,N'*-Dialkylisoindigo Derivatives from 3-Indolyl-2-oxindoles with DDQ

Da Young Seo, Beom Kyu Min, Jae Nyong Kim*

Department of Chemistry, Chonnam National University, Korea

cis-*N,N'*-Dialkylisoindigo derivatives were synthesized for the first time by the reaction of 3-indolyl-2-oxindoles with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) in aqueous 1,4-dioxane. *cis*-Isoindigo derivatives were completely isomerized to the corresponding *trans*-isomers by heating the solution in short time.



Poster Presentation : **ORGN.P-107**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

The efficient way to synthesize 4-Chloropyrazole

Donghoon Jeong, Yeong-Gweon Lim*

4-6, Agency for Defense Development, Korea

4-Chloropyrazole is the precursor for synthesis of LLM-116(4-amino-3,5-dinitropyrazole) which is pyrazole-based energetic material having high density and insensitivity. Three synthetic methods for 4-Chloropyrazole have been investigated and all of them have been conducted. Among them, the method using NaOCl is efficient way to decrease production cost and increase yield and purity. In this study, modified synthetic method for preparation of 4-Chloropyrazole was elaborated. The resulting product was fully characterized by ^1H NMR, ^{13}C NMR, GC-MS and differential scanning calorimeter.

Poster Presentation : **ORGN.P-108**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

New One-Pot Selective Synthesis of Diaryl Sulfoxides and Diaryl Sulfones via Visible-Light-Induced Silver-Catalysis

Juyoung Lee, Anna Lee^{1,*}

Department of chemistry, Myungji University, Korea

¹*Department of Chemistry, Myongji University, Korea*

Aryl sulfoxides and aryl sulfones are useful building blocks of various organic compounds and drug candidates and have exhibited many significant biological activities. Therefore, various methods for the synthesis of these compounds have been widely studied. The most conventional method for the synthesis of sulfoxides and sulfones is through the oxidation of sulfides. Many other synthetic approaches include the sulfonylation of arenes using strong acids, nucleophilic substitution of electrophilic sulfoxide derivatives and transition metal catalyzed arylation of sulfenate anions. However, these methods have drawbacks such as the use of stoichiometric amounts of oxidants and toxic and/or sensitive catalysts or reagents in the reactions. Herein, we report a new one-pot method for the selective synthesis of diaryl sulfoxides and diaryl sulfones via visible-light-induced silver catalysis under air. This novel and simple method did not require preactivation of the starting compounds and various aryl thiols were employed in the reaction successfully.

Poster Presentation : **ORGN.P-109**

Organic Chemistry

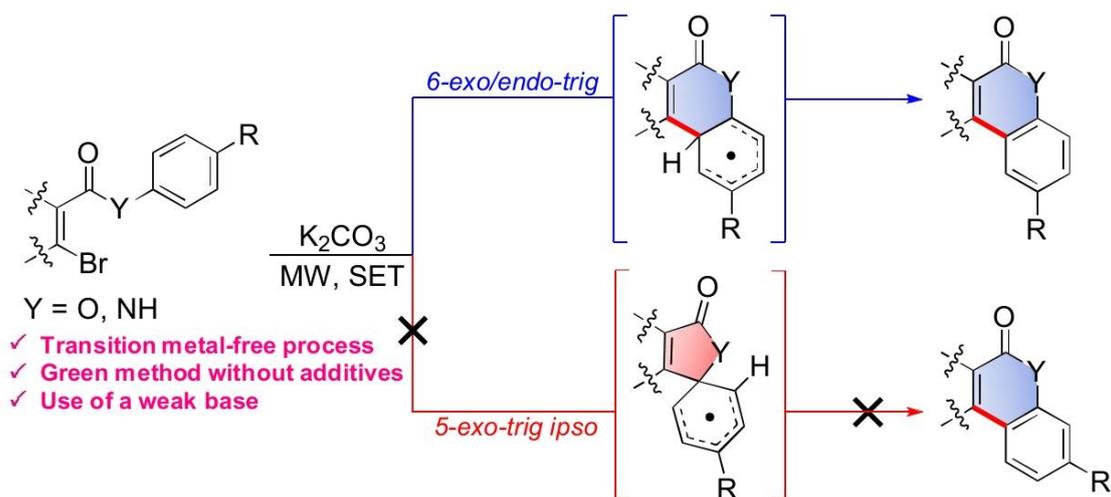
Grand Ballroom, THU 11:00~12:30

Microwave-Assisted Lactonization and Lactamization under Mildly Basic Conditions

Pham Duy Quang Dao, Chan Sik Cho*

Department of Applied Chemistry, Kyungpook National University, Korea

Aryl 2-bromobenzoates and aryl 2-bromocyclohex-1-enecarboxylates are cyclized by microwave irradiation in dimethylformamide in the presence of K_2CO_3 to give the corresponding 6H-benzo[c]chromen-6-ones and their 7,8,9,10-tetrahydro-analogs, respectively, in 50-72% yields. N-Aryl- β -bromo- α,β -unsaturated amides and N-aryl-2-bromobenzamides are also converted into quinolin-2(1H)-ones and phenanthridin-6(5H)-ones under the employed conditions.



Poster Presentation : **ORGN.P-110**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Pyrimidine- and Quinazoline-Fused Benzimidazole-4,7-diones Using Combinatorial Cyclocondensation and Oxidation

Dongyoung Kim, Pham Duy Quang Dao, Chan Sik Cho*

Department of Applied Chemistry, Kyungpook National University, Korea

β -Bromo- α,β -unsaturated aldehydes and 2-bromobenzaldehydes react with 4,7-dimethoxy-1H-benzo[d]imidazol-2-amine by microwave irradiation in DMF in the presence of a base to give the corresponding dimethoxy-substituted benzo[4,5]imidazo[1,2-a]pyrimidines and benzo[4,5]imidazo[1,2-a]quinazolines, respectively, in moderate to good yields. Oxidation of such N-fused hybrid scaffolds with aqueous ceric ammonium nitrate affords pyrimidine- and quinazoline-fused benzimidazole-4,7-diones in high yields.



Poster Presentation : **ORGN.P-111**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A study on synthesis of 1,3-Indanedione from phthalic anhydride

HwiJeong Won, SeungYun Baek, Byeong-Kwan An*

Department of Chemistry, The Catholic University of Korea, Korea

1,3-Indanedione [1H-indene-1,3(2H)-dione] which is an important cyclic-diketone molecules has been widely utilized as a key compound for the synthesis of drugs, forensic agents and opto-electronic dyes. In this study we investigated various synthetic methods for 1,3-indanedione from phthalic anhydride by using different reagents and report efficient synthetic routes to 1,3-indanedione.

Poster Presentation : **ORGN.P-112**

Organic Chemistry

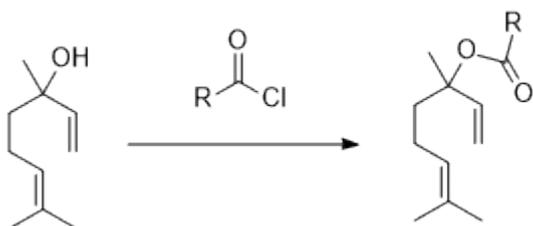
Grand Ballroom, THU 11:00~12:30

The Convenient Preparation of Linalool Derivatives; Applications of Aroma Chemicals

Min Ji Hong, JiEun Lee, Chujin Ahn*

Department of Biology and Chemistry, Changwon National University, Korea

The linalool derivatives have been used as aroma chemicals. The known and new linalool derivatives were prepared conveniently in our lab, and We investigated fragrance of the prepared linalool derivatives.



Poster Presentation : **ORGN.P-113**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

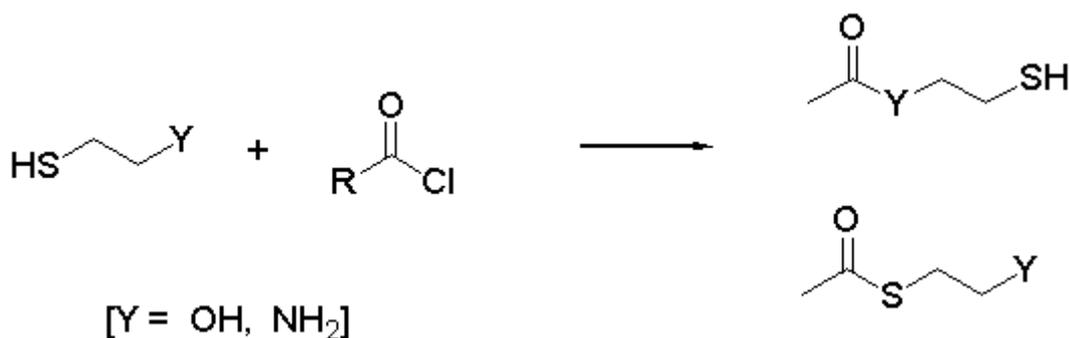
The Investigation of Chemoselectivity between S-Acylation and N-Acylation of β -mercaptoamine with Acid Chloride

Myeong Shin, Chujin Ahn^{1,*}

Changwon National University, Korea

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

The chemoselectivity is important to control functionalization in a molecule. In this research, 1) we investigated the selectivity between S-acylation and O-acylation depending on reaction condition with acid chloride and mercaptoethanol. 2) We investigated the selectivity between S-acylation and N-acylation depending on reaction condition with acid chloride and mercaptoamine.



Poster Presentation : **ORGN.P-114**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

An Easy Conversion of 2-Diphenylmethoxypyridine to Diphenylmethyl Esters Catalyzed by Boron Trifluoride·Diethyl Etherate

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

The diphenylmethyl (DPM) group commonly uses as a protecting group for carboxylic acids and has been used in a wide range of organic reactions and in pharmaceuticals. Hence, developing new practical synthetic method for DPM esters is important in organic chemistry and pharmaceutical chemistry. Herein, we report a direct method for preparation of DPM esters from 2-diphenylmethoxypyridine. In this study, small amount of boron trifluoride-diethyl etherate allowed 2-diphenylmethoxypyridine to make a complex which easily underwent direct transformation of carboxylic acids to DPM esters at room temperature. With boron trifluoride-diethyl etherate catalyzed conditions, this protocol showed to be highly effective for the preparation DPM esters from various carboxylic acids, and offers an efficient and applicable approach for facile esterification using catalytic boron trifluoride-diethyl etherate.

Poster Presentation : **ORGN.P-115**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Photochromic Reaction of Spiropyran-Picoline Dyad

Yejin Yu, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

Spiropyran (SP) is the most widely studied photo-switchable compound and has two heterocyclic rings connected by a spiro carbon. Upon exposure to UV light, Spirocarbon-oxygen bond of the colorless and non-fluorescent SP structure is broken to form the planar zwitterionic merocyanine (MC) structure with a blue or violet color in solution. The MC structure returns to the original SP structure thermally or on exposure to visible light. A new spiropyran derivative containing picoline ring, Spiropyran-Picoline dyad, was designed and synthesized. Photochromic reaction between Spiropyran-Picoline and Merocyanine-Picoline has been investigated by ultraviolet-visible absorption and fluorescence spectroscopic measurements.

Poster Presentation : **ORGN.P-116**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Colorimetric and Fluorometric Metal Cation Detection of Rhodamine-Quinoline Dyad

Heewon Choi, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

Rhodamine dyes show strong absorption and fluorescence in the visible region and can thus be detected easily and inexpensively with instruments called spectrofluorometers. Rhodamine dyes are used extensively in chemical and bio-technological applications such as fluorescence correlation spectroscopy, fluorescence microscopy, flow cytometry, and ELISA(enzyme-linked immunosorbent assay). Spirolactam ring form of rhodamine is colorless and non-fluorescent. On the other hand, ring-opened amide form of rhodamine is pink-colored and orange fluorescence. We report here a new rhodamine-based colorimetric/fluorometric sensing probe for the selective detection of metal cation. Rhodamine-Quinoline dyad has been prepared and characterized by IR, ¹H NMR, and ¹³C NMR spectra. Based on the absorption and fluorescence spectroscopic techniques, its metal cation sensing ability has been investigated.

Poster Presentation : **ORGN.P-117**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Metal Cation Detection Based on Rhodamine-Coumarin Dyad

Yeji Na, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

Rhodamine dyes have always received high-level attention because of their excellent photostability, water-solubility, intense color, and high absorption coefficient, strong striking orange fluorescence(570~590 nm) in the visible region. In recent years, selective optical receptors for the detection of metal cations using rhodamine derivatives have received extensive attention for designing and developing the colorimetric and fluorometric chemosensors. Coumarin is a fragrant organic compound in the benzopyrone chemical class. It is a natural substance found in many plants, and a colorless crystalline substance in its standard state. Coumarin, the water soluble and blue fluorescent (410~470 nm) dye, is used as a gain medium in some dye lasers, and as a sensitizer in older photovoltaic technologies. Combining two fluorescent dyes of rhodamine and coumarin is expected to exhibit very interesting physical and chemical properties. We report here a rhodamine-coumarin dyad as a candidate of chemosensor for a specific metal cation.

Poster Presentation : **ORGN.P-118**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Photoinduced Proton Release Reaction and Metal Cation Sensing of Sulfonate-functionalized Merocyanine Photoacid

Goeun Choi, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

Irreversible photoacids releasing a strong acid upon photolysis are mainly used as initiators and resists. Reversible photoacids that exhibit stronger acidity in the excited state than in the ground state show the disappearance of the proton accumulation when light irradiation is switched-off. In order to accumulate large amount of protons under low power continuous irradiation and despite very short lifetimes (1~100 ns), their proton release must be coupled with a slow isomerization process. In polar acidic medium, sulfonate-functionalized protonated merocyanine MEH-SO₃⁻ ($\Phi_T=0.37$ in DMSO, pK_a=7.8) behaves like long-lived reversible photoacids and attracts great interest for the pH-responsive light-controlled proton transfer reaction. MEH-SO₃⁻ photoacid undergoes a cyclization reaction under visible light to form highly acidic, sulfonate-functionalized protonated spiropyran SPH-SO₃⁻, and then a sulfonate-functionalized deprotonated spiropyran SP-SO₃⁻. In the dark, the reverse reaction from SP-SO₃⁻, to SPH-SO₃⁻, and then MEH-SO₃⁻ was observed. In this study, metal cation sensing as well as reversible proton-release/proton-capture photochromic reaction has been investigated at various pH and UV or visible light on/off conditions using absorption and fluorescence spectroscopy.

Poster Presentation : **ORGN.P-119**

Organic Chemistry

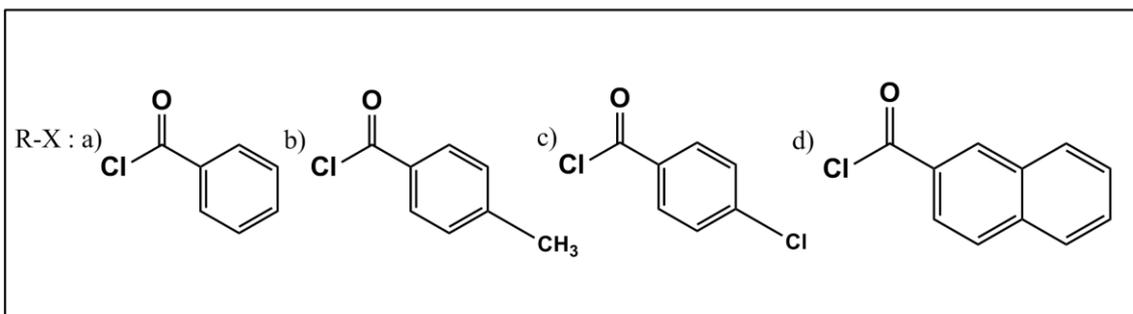
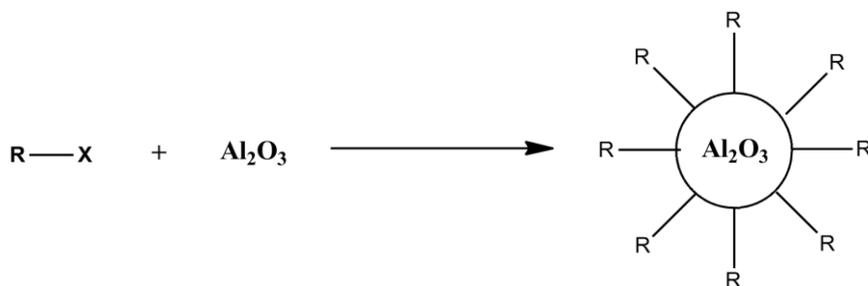
Grand Ballroom, THU 11:00~12:30

Organic Functionalization of Alumina: Luminescence Properties

Yongcheol Jung, Chujin Ahn*

Department of Chemistry, Changwon National University, Korea

Although several reactions of phosphoric derivatives with alumina have been reported, the other organic functional groups do not have been used for grafting organic moieties on alumina. In our lab, the hybrid material grafting organic moieties on alumina were prepared through the microwave irradiation or reflux and their photoluminescence (PL) properties were investigated



Poster Presentation : **ORGN.P-120**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

BODIPY-Based Electrochemiluminescent Probes for Rapid Detection of Hydrogen Peroxide

Yon Namkoong, Jong-in Hong^{1,*}

Department of Chemistry, Seoul National University, Korea

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

Here we report efficient electrochemiluminescent (ECL) probes (Probe **1**, **2** and **2F**) for hydrogen peroxide (H₂O₂). H₂O₂, generated through various metabolic pathways in biological systems, acts as a signaling molecule. As one of the reactive oxygen species, H₂O₂ is well known for its cytotoxicity at its abnormal concentration, which causes oxidative stress in cells and results in cellular damages. Our probes showed remarkable sensitivity and selectivity toward H₂O₂ with their high turn-on luminescence ratio and adequate reactivity. The BODIPY cores of probe **2** and **2F** are fully substituted with alkyls to improve the stability of radical species generated during the ECL process, which is not assured with the unsubstituted positions in probe **1**. As a result, probe **2** and **2F** provided ECL turn-on response to H₂O₂ with tripropylamine as a reductive co-reactant in an aqueous organic cosolvent. Furthermore, we reduced pK_a of the recognition unit by fluorination (probe **2F**) for rapid detection. Bright ECL was observed after 30 min incubation of probe **2F** with H₂O₂ while it took 1 hour for probe **2**. Although numerous ECL luminophores were reported based on BODIPY, there are only a few cases of BODIPY-based ECL sensors. Our study demonstrates the possibility of BODIPY dyes for detection of meaningful biotargets such as H₂O₂ utilizing ECL.

Poster Presentation : **ORGN.P-121**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Efficient Direct DBU-Catalyzed Aminolysis of Trichloroethyl Esters

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

A direct aminolysis of 2,2,2-trichloroethyl esters in the presence of a catalytic amount of DBU is presented. The 2,2,2-trichloroethyl group is known to be a desirable protecting group for carboxylic acid and also easily cleaves. A series of organic reagent was screened to prepared amides from trichloroethyl esters, and it was found that the direct syntheses of amides were easily achieved in high yield when a catalyzed amount of DBU was employed. This reaction procedure showed to be an efficient method to synthesize a series of amide compounds from primary and secondary amines in high yield, suggesting a highly effective direct one-pot synthesis of amide compounds from 2,2,2-trichloroethyl esters in the presence of DBU catalyst.

Poster Presentation : **ORGN.P-122**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Rapid Boron Trifluoride·Diethyl Etherate-Mediated Transformation of *tert*-Butyl Esters from 2-*tert*-Butoxypyridine

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Tert-butyl ester is a structure that has possessed many advantages in organic synthesis because of the stability of the ester to nucleophilic attack and its easy cleavage. Here, we develop a fast direct transformation of *tert*-butyl esters from 2-*tert*-butoxypyridine. The employment of boron trifluoride-diethyl etherate in toluene solvent increased the rate of reaction at room temperature and rapidly achieved the *tert*-butyl esters. Using this method, a series of *tert*-butyl esters were prepared from various carboxylic acids in high yields. This novel, efficient, and applicable procedure showed to be a promising and effective method for the protection of carboxylic acids in a broad range of organic syntheses.

Poster Presentation : **ORGN.P-123**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

More Stable Bimolecule State by Strong Intermolecular Hydrogen Bonds of a Naphthalene Urea Derivative

Ga Eun Lee, Young Ju Lee¹, Jin Yong Lee², Kye Chun Nam^{3,*}

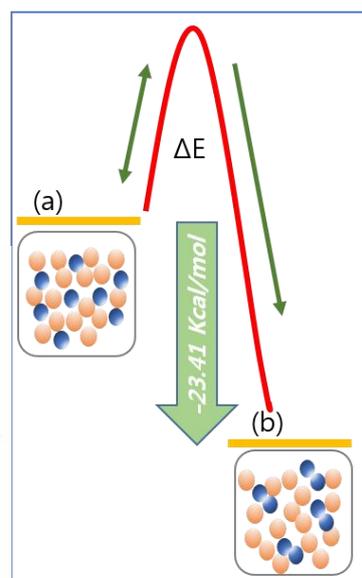
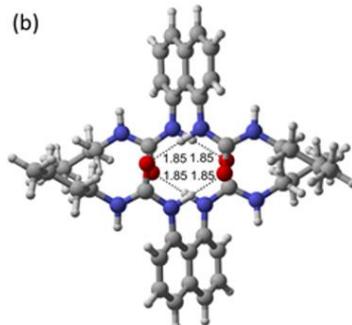
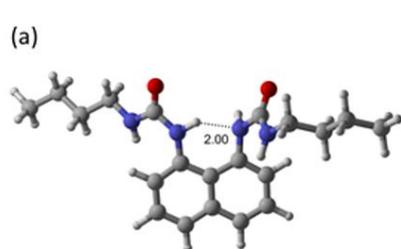
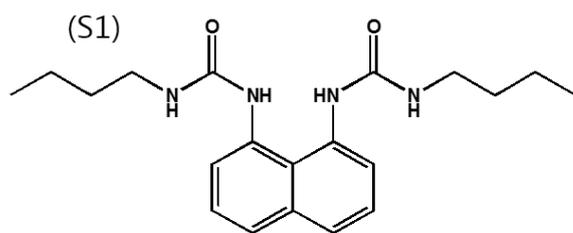
chemistry department, Chonnam National University, Korea

¹*Korea Basic Science Institute, Korea*

²*Department of Chemistry, Sungkyunkwan University, Korea*

³*Department of Chemistry, Chonnam National University, Korea*

Naphthalene urea derivative(S1) developed as a fluorine sensor showed unusually the slow exchange between a monomer(a) and a dimer(b) in DMSO solution. We found that both (a) and (b) state substances coexisted on the ¹H NMR spectrum at room temperature. Higher values of concentration and temperature increased the portion of (b) state. Through the computational methods, we could calculate the most stable configuration by four same strong hydrogen bonds as shown below (b), which binding energy was -23.41 Kcal/mol. These hydrogen bonds make the dimer molecule perfectly symmetrical to form, and so that only two sets NH peaks are formed which is so different from monomer molecule. From NMR spectra and calculation results, we ascertained the bimolecular structure is more likely to form to the lower energy state as temperature and concentration increase. Further study of sensing properties of dimer molecules is underway. The relevant investigations of sensing properties of dimer-molecules is in progress.



Poster Presentation : **ORGN.P-124**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Platinum(IV)-catalyzed 1,3-aryl migratory reactions of 2,3-diaryl indole from *ortho*-alkynyl-*N*-aryl-*N*-sulfonamides

Dong Yun Kang, Khyarul Alam, Jin Kyoong Park*

Department of Chemistry, Pusan National University, Korea

Indole is an aromatic two-ring heterocyclic compound possessing potent biological activity. In particular, 2,3-diaryl indoles have been reported to have anti-cancer activity in several studies. The reason why there are many methods available for synthesizing various 2,3-disubstituted indoles, one of which is an intramolecular cyclization of *ortho*-alkynyl-*N,N*-disubstituted amides. Most of these intramolecular cases for the synthesis of 2,3-disubstituted indoles involves functional group migration strategy using transition metal catalysts through selective migration of a particular function group. Although, sulfonyl, acyl and allyl groups have been known to undergo such type of reaction, aryl migration is not studied yet. Herein, we describe a PtCl₄-catalyzed 1,3- aryl migratory reaction of *ortho*-alkynyl-*N*-aryl-*N*-methylsulfonyl amide derivatives that affords 1-(methylsulfonyl)-2,3-diphenyl-1*H*-indole in reasonable yields. The practicability of the current transformation was also verified by synthesizing twenty different disubstituted indoles in reasonable yields.

Poster Presentation : **ORGN.P-125**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Ratiometric Hydrogen Peroxide Probe Producing Solid Form of Product in Cell

Hye Rim Kim, Kyo Han Ahn*

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

In biological system, hydrogen peroxide (H_2O_2), which is produced from the mitochondria as the by-product of aerobic respiration, maintains certain concentration and plays roles as an oxidative stress marker and a messenger in cellular signal transduction. Homeostasis failure of H_2O_2 in mitochondria is connected with various diseases, such as diabetes, neurodegenerative disease, cancer. Therefore, there is a huge demand for developing tools to quantify H_2O_2 level in mitochondria selectively and sensitively. Even though some ratiometric H_2O_2 probes selectively localized in mitochondria have been reported, there is limitation on sensitive detection of H_2O_2 because of unreacted probes remaining in cell which give rise to the interference with signal of product. To address the issue, we have disclosed designed the ratiometric H_2O_2 probe producing the solid form of products in cell. Solid form of products is strong resistance of diffusion, which is well localized, and it is possible to sensitively detect the H_2O_2 , allowing the unreacted probe to be washed.

Poster Presentation : **ORGN.P-126**

Organic Chemistry

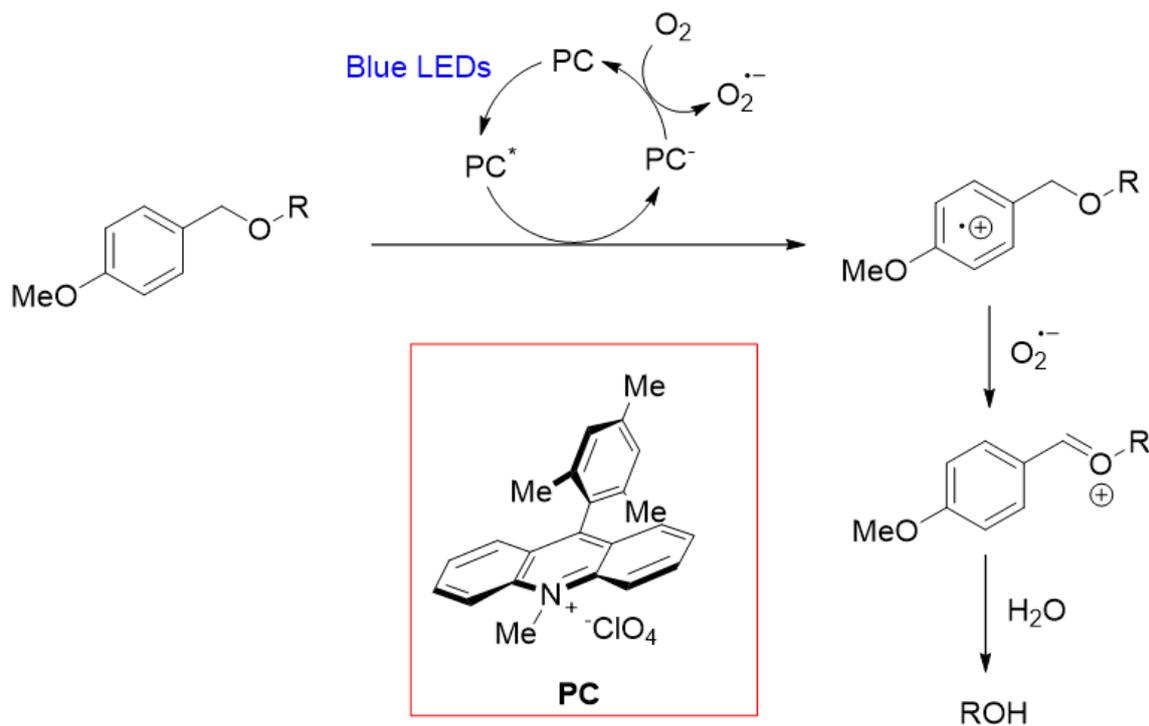
Grand Ballroom, THU 11:00~12:30

Mild Deprotection Method for p-Methoxybenzyl Ether via Photoredox Catalysis

Deok Kyun Ahn, Sang Kook Woo*, Young Woo Kang

Department of Chemistry, University of Ulsan, Korea

We developed visible-light photoredox catalyzed deprotection of the p-methoxybenzyl(PMB) protecting group using 9-mesityl-10-methylacridinium perchlorate as photoredox catalyst and air as the terminal oxidant. This method is highlighted by excellent functional group tolerance, protecting group orthogonality, mild reaction conditions.



Poster Presentation : **ORGN.P-127**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of peptide nucleic acid using fully protected PNA trimers

Alagarsamy Periyalagan, Ji Hye Park¹, In seok Hong^{1,*}

Department of chemistry, Kongju National University, Korea

¹Department of Chemistry, Kongju National University, Korea

Solid phase peptide synthesis is the most common method of synthesizing peptide nucleic acid (PNA) by sequential coupling of the corresponding monomers. However, when synthesizing a long oligomer or synthesizing an oligomer having a certain continuous base sequence, the final synthesis yield is limited. To overcome these limitations, we first report the synthesis of PNA oligomers using fully protected PNA trimers instead of monomers. Fully protected PNA trimer blocks were prepared by solution phase synthesis. In the case of oligomer synthesis using trimer block, the number of synthesis cycles can be reduced by about 66%, so that the synthesis time can be reduced and relatively high purity oligomers can be synthesized.

Poster Presentation : **ORGN.P-128**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Crystal Structures of dibenzylpyromellitic diimide and dibenzylpyromellitic dithioimides

Hansu Im, Juhyeon Park, Tae Ho Kim, Tae Ho Kim*, Jineun Kim*

Department of Chemistry, Gyeongsang National University, Korea

Dibenzylpyromellitic diimide (**1**) was synthesized by the reaction of pyromellitic dianhydride with 2-phenylethylamine, and dibenzylpyromellitic dithioimides (**2**) was prepared by thionation of **1** with Lawesson's reagent. Two compounds were confirmed to be composed of a terminal benzyl group and central pyromellitic diimide and pyromellitic diimide substituted with S atom, respectively with single crystal X-ray diffraction. **1** and **2** lie on a crystallographic inversion center. The phenyl groups of **1** and **2** are tilted by 72.97° and 72.69° with respect to the plane of the central arene ring, forming an elongated S-shaped conformation. **1** is connected *via* weak C—H···O hydrogen bonds and C—H··· π interactions. **2** is connected by C—H··· π interactions and weak short S···S contacts. **1** and **2** form supramolecular two-dimensional layers extending parallel to the *ab* plane.

Poster Presentation : **ORGN.P-129**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Ratiometric Near IR Probe Based on Glucosylated Heptamethinylcyanine for In Vivo Imaging of Nitroreductase

Won joo Lee, Hae-Jo Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Background: Nitroreductase (NTR) is activated in such a hypoxic condition as cancer. Therefore, the detection of hypoxic NTR is a feasible tool for the diagnosis of tumor cells, warranting robust detection for a variety of biological studies.^{1,2}**Materials and Method:** Chemical probes were prepared according to the standard method in the lab and NTR enzyme together with NADH was purchased from the chemical suppliers.**Result:** A Cy7-based dual optical probe was developed for selective and sensitive detection of NTR in a NIR fluorescence region.³ The probe exhibited dramatic optical changes with strong fluorescence ($F/F_0 = 9.0$ at λ_{em} 747/807 nm) as well as intense blue color by the nitro-to-amine functional group transformation and displayed a very low limit of detection of NTR in PBS buffer. Further application of the probe to endogenous NTR was successfully applied in HeLa cells as well as a mouse model of breast cancer, exhibiting its preferential localization in the cellular mitochondria and heavy accumulation in the tumor tissues of living mice enough to obtain brighter tumor imaging through *i.v.* injection. **Conclusion:** Latent chromogenic and fluorogenic probe was successfully applied for the detection of mitochondrial NTR in vivo as well as in vitro.**References**¹ Xu, K.; Wang, F.; Pan, X.; Liu, R.; Ma, J.; Kong, F.; Tang, B. *Chem. Commun.*, **2013**, 49, 2554.² Li, Y.; Sun, Y.; Li, J.; Su, Q.; Yuan, W.; Dai, Y.; Han, C.; Wang, Q.; Feng, W.; Li, F. *J. Am. Chem. Soc.*, **2015**, 137, 6407³ Chin, J.; Kim, H.-J. *Coord. Chem. Rev.*, **2018**, 354, 169

Poster Presentation : **ORGN.P-130**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Coordination-driven self-assembly of tetrafluoro analog of 1,4-bis(4-pyridylethynyl)benzene with arene ruthenium acceptors

Donghwan Kim, Jatinder Singh, Kiwhan Chi*

Department of Chemistry, University of Ulsan, Korea

In recent years, coordination-driven self-assembly has become a dominant method for constructing complex supramolecular topologies. These supramolecular architectures are fascinating because of their functional and structural beauty. Our group have reported a number of complex molecular topologies such as Solomon links, Borromean rings, and Hopf's links using coordination-driven self-assembly. Boromean rings were obtained by the coordination-driven self-assembly of dipridyl donor, 1,4-bis(4-pyridylethynyl)benzene and tetracene based Ru(II) acceptor. Since, application and results of the self-assembled architectures can be improved by modifying the donor and acceptor building blocks. Herein, we report the coordination-driven self-assembly of 1,4-bis(4-pyridylethynyl)tetrafluorobenzene donor with various arene ruthenium acceptors.

Poster Presentation : **ORGN.P-131**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

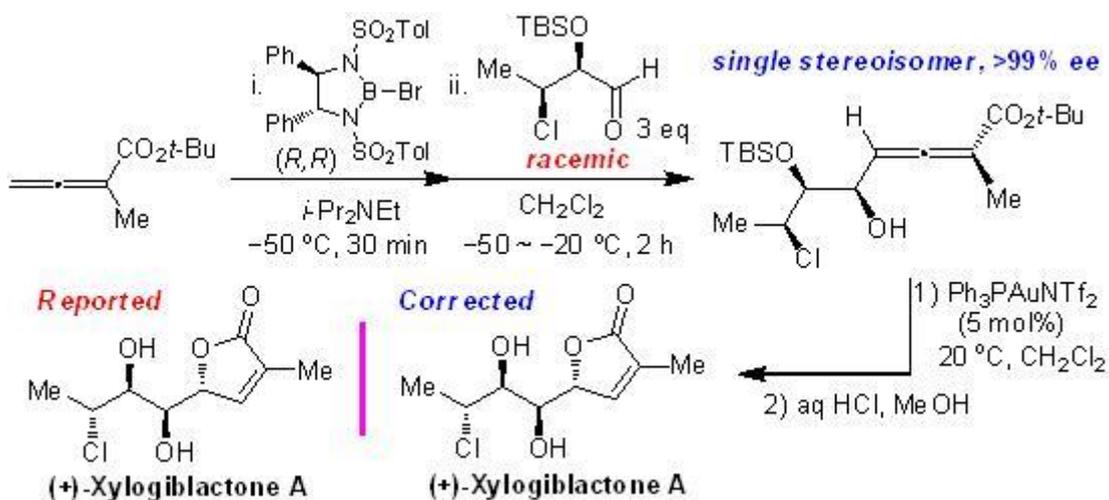
A Highly Effective Kinetic Differentiation of Racemic Aldehydes by Allenoate Aldol Reaction: Correction of Stereochemistry for (+)-Xylogibactone A

Saehansaem Park, Heejung Jeong, Ahhyeon Hong¹, Jimin Kim*, Chan-Mo Yu^{1,*}

Department of Chemistry, Chonnam National University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

Recently, we disclosed our discovery of a highly stereoselective synthesis of unusual gamma aldol adducts from the reaction of 2-alkyl allenoates with a chiral bromoborane in the presence of Hunig base, and then aldehydes. We have developed a method for the kinetic resolution of racemic aldehydes to increase practicability. This simple laboratory process can also be operated in parallel and provides rapid access to gamma aldol adducts in pure form. As a synthetic application, we undertook an enantiospecific synthesis of (+)-xylogibactone A. However, spectral data including NMR data did not match with the literature. We present herein our recent investigations for the synthesis of (+)-xylogibactone A and related natural products to correct stereochemical relationship.



Poster Presentation : **ORGN.P-132**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

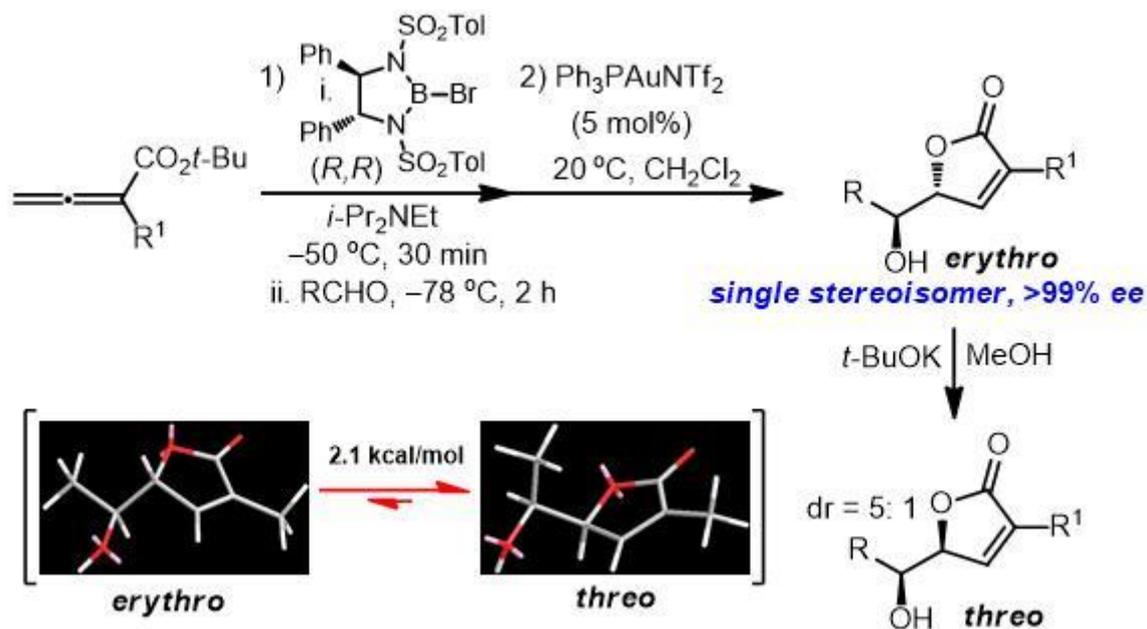
A Conversion of erythro-5-(1-hydroxyalkyl)-furan-2(5H)-ones to threo-Diastereomers under Basic Epimerization Conditions

Gyungah Pak, Weonju Yu, Dongeun Kim¹, Chan-Mo Yu^{1,*}, Jimin Kim^{*}

Department of Chemistry, Chonnam National University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

During the past few decades, substantial progress has been made for a variety of diastereoselective methods mediated by chiral reagents and catalysts. Nonetheless, only a limited number of methods exist to establish both diastereomers selectively, despite their plentiful synthetic potential. Recently, we have disclosed a new method for the stereospecific synthesis of furanone derivatives via two step sequence: asymmetric allnoate aldol and gold cyclization as described below. During the investigations, we observed that erythro isomer can be converted to the corresponding threo-diastereomer. We would like to present herein reaction conditions, scope and limitation of the reaction, and its synthetic applications to bioactive substances.



Poster Presentation : **ORGN.P-133**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A fused oxazolidinoindole-based dual optical probe for nitroreductase with dramatic chromogenic and fluorogenic changes

HyunSeok Seo, Hae-Jo Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Background : Biomedical studies indicate that the hypoxic status of solid tumors is closely related to the process of tumor progression. Therefore, the development of efficient methods for detecting the hypoxic conditions in living systems is very important for biomedical research. Nitroreductase (NTR) is activated in a hypoxic condition such as cancer cells so the detection of hypoxia and NTR is a feasible tool for the diagnosis of tumor cells and warrants robust detection for a biological study.^{1,2,3,4,5}**Materials and Method**: Chemical probe was prepared according to the standard method in the lab and NTR enzyme together with NADH was purchased from the chemical suppliers.**Result**: A fused oxazolidinoindole-based dual optical probe was developed for detection of NTR. Upon addition of NTR in the presence of NADH, the probe exhibited dramatic optical changes with strong fluorescence ($F/F_0 = 14$, λ_{em} 580 nm) as well as intense orange color (λ_{abs} 460 nm) by a nitro-to-amine functional group transformation and displayed a very low limit of detection (LOD = 10.4 ng/mL) of NTR in PBS buffer. And it also showed selectively detection of NTR in inhibitor assay with Dicoumarol. Further application to endogenous cellular NTR was successfully applied in A549 cells.**Conclusion** : Latent colorimetric and fluorometric probe was successfully applied for the detection of endogenous cellular NTR in vivo as well as in vitro.**References**¹Padhani, A. R.; Krohn, K. A.; Lewis, J. S.; Alber, M. *Eur. Radiol.* **2007**, *17*, 861.²Brown, J. M.; William, W. R. *Nat. Rev. Cancer*, **2004**, *4*, 437. ³Wilson, W. R.; Hay, M. P. *Nat. Rev. Cancer*, **2011**, *11*, 393.⁴Harris, A. L. *Nat. Rev. Cancer*, **2002**, *2*, 38 - 47.⁵Chen, Y.; Hu, L. *Med. Res. Rev.* **2009**, *29*, 29.

Poster Presentation : **ORGN.P-134**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Improvements for dehalogenation via organic photoredox catalyst

Doyon Kim, Yonghwan Kwon, Varun Singh, Min Sang Kwon*

Department of Materials Science Engineering, Ulsan National Institute of Science and Technology, Korea

Abstracting halide atoms from organohalide compounds and subsequently generating free-radical to produce reactive intermediates have proven to be important step in chemical synthesis. Hence, many scientists have thrived to improve this dehalogenation process to more efficient, simple, and environmentally friendly way. Adoption of photocatalytic process was proven to be promising, as it is inexpensive and sustainable way to induce chemical reactions. It is widely known to utilize inorganic photocatalysts such as iridium or ruthenium complexes in dehalogenation. However, their potential hazards and toxicity were of concerns thus many researches were done to make use of organic photocatalysts. Nevertheless, still there have been limitations such as UV-light irradiation for the activation of catalysts, requisites for harsh condition, or difficulties in reducing electron-rich aryl halides. So here in we present purely organic photocatalyst designed, which successfully demonstrates facile dehalogenation in mild conditions for the most aryl halides including even aryl chlorides and electron-rich aryl bromides, which have so far been reported to be difficult to reduce.

Poster Presentation : **ORGN.P-135**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Understanding of Rh(III)-Catalyzed 7-Azaindole Synthesis: Origin of Regioselectivity and Identifying Directing Groups Impacting on Intermolecular Heterocyclization

Ho Ryu, Dasol Cho, Sungwoo Hong*, Mu-Hyun Baik*

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

7-Azaindole is a useful molecule in industry and pharmacy as a molecular scaffold. The two nitrogen atoms on the molecule introduce enhanced bioactivity compared to the corresponding indole. Although a facile method to synthesize the 7-Azaindoles has been devised by Hong et al., understanding the detailed mechanism was not fully accomplished. To rationalize the mechanism of the synthesis for 7-Azaindole, we commenced computational simulation based on density functional theory (DFT). We found that the C–H bond activation on the ortho-position of the amidopyridines takes place via concerted metalation deprotonation. A proton transfers from the sp²-carbon of the pyridine ring to the bicarbonate, which subsequently yields water and carbon dioxide. The Gibbs free energy from this decomposition makes the reaction to be more thermodynamically favorable as providing the significant driving force. When we figured out the molecular interaction in the alkyne insertion step, which is determining the regioselectivity, we realized that the carbon next to the phenyl group in the alkyne has a more favorable orbital symmetry to interact with the rhodium center. To intimately explain the phenomenon, we have additionally introduced a distortion-interaction analysis that quantifies the hardness and softness of the interactions between two substrates. As precisely describing the molecular orbital interaction, we elucidated that the orbitals of the alkyne in the fast reaction coordinate can be efficiently overlapped with d-orbital of the rhodium center. We are trying to regulate the regioselectivity to afford the 2-, 3- groups reversed 7-Azaindole product and redesign the synthesis to generate 1,8-naphthyridines by modifying the substrates or substituting the metal and coordinated ligands.

Poster Presentation : **ORGN.P-136**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Self-assembly of interlocked ruthenium(II) metallacages

Jatinder Singh, Donghwan Kim, Kiwhan Chi*

Department of Chemistry, University of Ulsan, Korea

In recent years, coordination-driven self-assembly has become a dominant means of constructing functionalized metallocsupramolecular architectures with promising biological, electronic, and photophysical properties. Coordination-driven self-assembled container molecules have attracted particular attention owing to their numerous potential applications such as containers for labile chemical species, molecular flasks for chemical reactions and transport vehicles for drug molecules. In this poster, we report the coordination-driven self-assembly of triazole based donors with various arene ruthenium acceptors and the potential applications. All the new metallocsupramolecules have been characterized by elemental analysis, ^1H NMR, ^{13}C NMR and mass spectrometry.

Poster Presentation : **ORGN.P-138**

Organic Chemistry

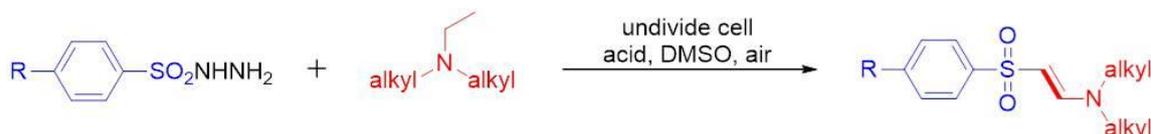
Grand Ballroom, THU 11:00~12:30

Electrochemical Reaction: Synthesis of Vinyl Sulfones using Multi-Channel ElectroChem

Han-Sung Kim, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

The synthesis of vinyl sulfones has attracted much attention due to their biological activities, antithyroid drugs, or hypoglycemia. Vinyl sulfones are important intermediates and reagents for the synthesis of organic compounds. Given the importance of vinyl sulfones, we need to develop more synthetic methods to meet the needs of such compounds. Here, we introduce a state-of-the-art electrochemical strategy in which a mild and practical route to vinyl sulfones has been developed based on the reaction of the tertiary aliphatic amines with aryl sulfonyl hydrazide by electrolysis in moderate yield.



Poster Presentation : **ORGN.P-139**

Organic Chemistry

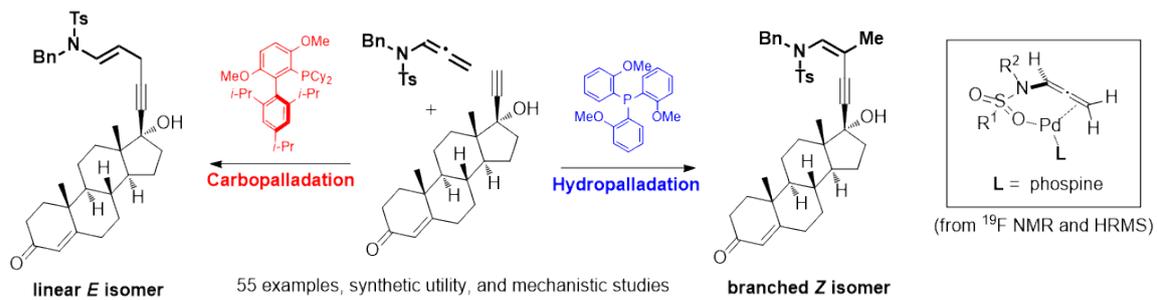
Grand Ballroom, THU 11:00~12:30

Regiodivergent Synthesis of 1,3- and 1,4-Enynes via Kinetically Favored Hydropalladation and Ligand-Enforced Carbopalladation

Tapas Ranjan Pradhan, Jin Kyoong Park*

Department of Chemistry, Pusan National University, Korea

In continuation of our recent research on ynamides, we reported herein, a regio- and stereoselective hydroalkynylations of a readily available allenic skeleton, *N*-sulfonyllallenamide. Although, hydroalkynylations were successfully applied to electron-neutral/electron-deficient cumulene (allenoates and allenylphosphine oxides), regiodivergent and stereoselective alkynylation is a significant challenge, since the two contiguous reactive π -systems are prone to isomerization and may afford a mixture of regio- and very often, stereoisomers. In order to address the aforementioned challenges, we attempted to take advantage of the potential chelating amide group of the substrate for control of the stereoselectivity and to screen sterically and electronically differentiated phosphine ligands for the desired regiocontrol. Moreover, the present transformation represents a complementary, highly regiodivergent, and stereospecific cross-coupling approach for the syntheses of conjugated and skipped ynenamides promoted by two different ligands, using a single metal catalyst. Neighboring group chelation and phosphine-ligand selection were found to be crucial to develop a reaction that takes place under such mild conditions to allow easy modification of complex substrates such as steroids, carbohydrates, alkaloids, chiral ligands, and vitamins with a broad scope and excellent chemoselectivity. We also proposed reasonable mechanisms in which the ligand-controlled hydro- and carbopalladation processes in the current divergent reaction operate separately by the formation of σ -vinyl-Pd intermediate, based upon experimental results.



Poster Presentation : **ORGN.P-140**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Photoinduced Preparation of Alpha, beta-dibromo Ketones From Alpha-bromo ketones and N-bromosuccinimide

Da Yoon Moon, Bong Ser Park*

Department of Chemistry, Dongguk University, Korea

Preparation of α , β -dibromo carbonyl compounds has been attracting attention because they are utilized as useful intermediates in organic synthesis. The dibromo compounds can be used as precursors to synthesize α -bromoacrylates, vinyl azides, β -bromo carbonyl compounds, and etc. Also, if the preparation method is simple, it is possible that dibromo compounds can be utilized as convenient protecting groups of vinyl ketones. Because of its wide usage, it is well known that the dibrominated compounds can be easily obtained by the direct addition of Br_2 to vinyl ketones. However the use of molecular bromine is very hazardous. Therefore there has been a lot of effort to overcome this difficulty of using molecular bromine, but most required expensive reagents or were limited to specific structures. Recently, we reported a photoinduced 1,2-Br shift reaction of α -bromopropiophenones. We discovered α -bromopropiophenones can be converted into β -bromopropiophenones by photochemical C-Br cleavage reaction. It was suggested the reaction is occurred by the conjugate addition of HBr to the α β -unsaturated ketone intermediates formed by the C-Br bond cleavage initiated by photoreaction. We wondered if the photolysis of α -bromopropiophenones were done in Br_2 enriched condition, the α , β -unsaturated ketone intermediates could be trapped by Br_2 and give out α , β -dibromo ketones. It is well known that Br_2 can be formed by the reaction of N-bromosuccinimide (NBS) and HBr. Since HBr is one of the products of the 1,2-Br shift reaction, we assumed that α , β -dibromo ketones could be synthesized by the irradiation of α -bromopropiophenones in presence of NBS.

Poster Presentation : **ORGN.P-141**

Organic Chemistry

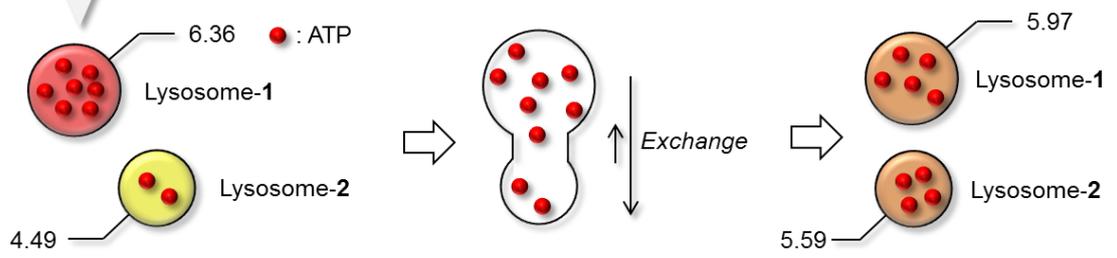
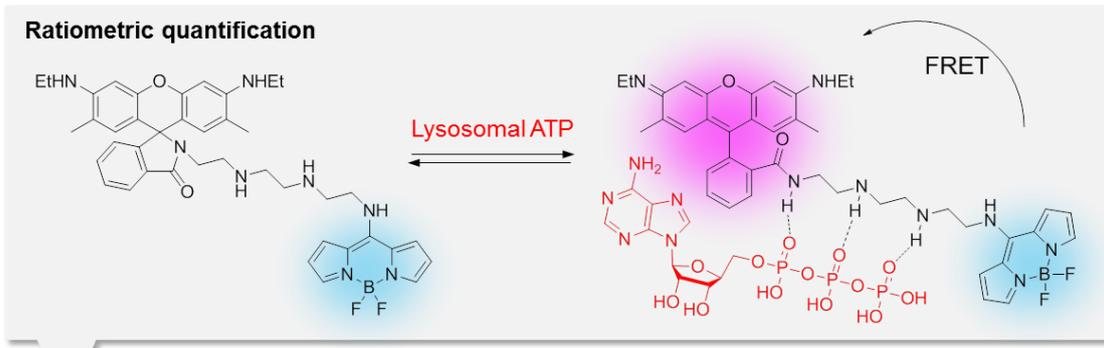
Grand Ballroom, THU 11:00~12:30

Direct *In Cellulo* Observation of Lysosomal Membrane Fusion Processes Using a Ratiometric Two-Photon Fluorescent Probe for Tracking Lysosomal ATP

Yong Woong Jun, Kyo Han Ahn*

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

Vesicles exchange their contents through membrane fusion processes, kiss-and-run and full-collapse fusion. Indirect observation of these fusion processes using artificial vesicles enhanced our understanding on the molecular mechanisms involved. Direct observation of the fusion processes in a real biological system, however, remains as a challenging task owing to many technical obstacles. In this seminar, we disclose a ratiometric two-photon probe offering real-time tracking of lysosomal ATP with quantitative information for the first time. By applying the probe to two-photon live-cell imaging technique, the lysosomal membrane fusion process in cells has been directly observed along with the quantitative information of endogenous ATP. Results show that the kiss-and-run process between lysosomes proceeds through repeated transient interactions with gradual content mixing, whereas the full-fusion process occurs at once. Furthermore, it is confirmed that both the fusion processes proceed with conservation of the content.



Real-Time Monitoring of Membrane Fusion

Poster Presentation : **ORGN.P-142**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and electroluminescent properties of platinum(II) complexes based on tetradentate pyridine containing ligands

Namhee Hwnag, Soyoung Pak, Soo Kyung Kang, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

In this study, two platinum(II) complexes based on tetradentate pyridine containing ligands were designed and synthesized. These materials could serve as phosphorescent dopants for organic light-emitting diodes (OLEDs). To investigate their electroluminescent (EL) properties, multilayered OLEDs were fabricated using synthesized materials as dopants in CBP host material.

Poster Presentation : **ORGN.P-143**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

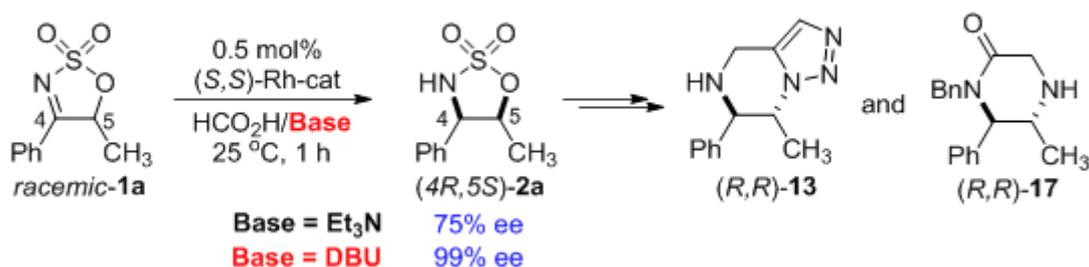
DBU-Promoted Dynamic Kinetic Resolution in Rh-Catalyzed Asymmetric Transfer Hydrogenation of 5-Alkyl Cyclic Sulfamidate Imines: Stereoselective Synthesis of Functionalized 1,2-Amino Alcohols

Hyeong Rae Kim, Raghavendra Achary¹, Hyeon Kyu Lee^{1,*}

Medicinal Chemistry, University of Science & Technology, Korea

¹*Korea Chemical Bank, Korea Research Institute of Chemical Technology, Korea*

Dynamic kinetic resolution (DKR)-driven asymmetric transfer hydrogenation of 5-alkyl cyclic sulfamidate imine produces the corresponding sulfamidate with excellent levels of diastereo- and enantioselectivity by employing a HCO₂H/DBU mixture as the hydrogen source in the presence of the Noyori-type chiral Rh-catalyst at room temperature for 1 h. In this process, DKR was induced by DBU-promoted rapid racemization of the substrate. Stereoselective transformations of the resulting cyclic sulfamidates to functionalized enantiomerically enriched 1,2-amino alcohol and chiral amine substances are also described.



Poster Presentation : **ORGN.P-144**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

New Approach for Selective 1-Alkylation of 5-Aminotetrazoles

Jiyu Kim, Yeong-Gweon Lim*

Agency for Defense Development, Korea

These days, high energy density materials (HEDMs) with 5-aminotetrazole (5-AT) core has been received attention due to its high nitrogen content, remarkable stability and low sensitivity. To synthesize effective HEDMs containing 5-AT core, selective alkylation on 1-position of 5-AT is considered as important step. However, there is no effective method to alkylate selectively at 1-position. Reported methods had limitations like low 1- and 2-position selectivity or using hazardous reagent such as BrCN. Here we introduce our new approaches to alkylate at 1-position of 5-AT : We form new alkyl ring using secondary amine at 1-position and primary amine at 5-position (amino group). Later, this alkyl ring will be cleaved to 1-alkylated-5-aminotetrazole.

Poster Presentation : **ORGN.P-145**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Computational study on the mechanism of boron-catalyzed reductive carbocyclization of homoallylic alcohols to syn-cyclobutanes

Jinhoon Jeong, Mu-Hyun Baik*, Sukbok Chang^{1,*}

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Catalyzed reductive carbocyclization of homoallylic alcohols using hydrosilanes as reducing reagents has been achieved to provide a variety of 1,2-disubstituted arylcyclobutanes with an excellent diastereoselectivity. In the proposed mechanism, there are three pathways for generating cyclobutane product. One involves a concerted nucleophilic borohydride attack to carbocation cyclobutane intermediate, which is but excluded on the basis of the kinetic isotope effect. The other two pathways of intramolecular carbocyclization differ from the perspective of whether the cyclopropane intermediate is involved. The deuterium labeling experiments show that the reaction may proceed via dual ring-closing pathway. Our density functional theory (DFT) calculations display that this dual ring-closing pathway would be reasonable.

Poster Presentation : **ORGN.P-146**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Thermally Cross-Linkable Styrene-Based Host materials for Organic Light-Emitting Diodes

Jae-Ho Jang, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

Thermally cross-linkable host materials containing carbazole, imidazole, and triphenylamine were designed and synthesized for solution-processed organic light-emitting diodes (OLEDs). The host materials with styryl groups can be thermally cross-linked by curing at 150-200 °C without any polymerization initiator. Excellent solvent resistance was observed for all the host materials. The highest occupied molecular orbital energy levels of 5.4-5.6 eV are estimated for these host materials, which indicates low injection barrier from the hole transport layer. A current efficiency of 5.3 cd/A, power efficiency of 3.2 lm/W, and external quantum efficiency of 3.6 % were achieved for solution-processed (MPHMQ)2Ir(tmd)-based OLEDs by using the thermally cross-linkable host material.

Poster Presentation : **ORGN.P-147**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Isothiouronium salt type organocatalysts for the Morita-Baylis-Hillman reaction

Sungmin Kang, Taek Hyeon Kim*

School of Chemical Engineering, Chonnam National University, Korea

New isothiouronium salt type organocatalysts have been developed for the Morita-Baylis-Hillman reaction. The isothiouronium salt type organocatalysts have better catalytic performance than the urea and thiourea type organocatalysts due to their strong hydrogen bonding ability. The Morita-Baylis-Hillman reaction using isothiouronium salt type organocatalysts were accomplished with high yield.

Poster Presentation : **ORGN.P-148**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A study on the reactions for four types of 1,2-benzisothiazol-3-one-1,1-dioxide anticipated biological activity

Seung Ryul Lee, Ju Hyun Song^{1,*}, Eon Jin Lee¹, Jungtai Hahn²

Dong-A University, Korea

¹*Department of Chemistry, Dong-A University, Korea*

²*Department of Beauty Care, UI University, Korea*

Saccharin is an artificial or non-nutritive sweetener. Humans can't break down saccharin, so it leaves the body unchanged. Alkylation methods to prepare N- and O-substituted(carbonyl oxygen) derivatives of 1,2-benzisothiazol-3-one-1,1-dioxide(saccharin) are well established and these have provided researchers with the straightforward synthesis of novel and potentially bioactive molecules. In addition to N- and O-alkylation, compounds derivative on the benzene moiety are particularly desirable. All type of saccharin derivatives would however present attractive properties for the development of new bioactive, drug-like small molecule compounds. We report reactions for four types of saccharin(saccharin, 2-hydroxymethylsaccharin, chloro saccharin, sodium saccharin). Synthesized saccharin derivatives will be executed evaluation of biological activity

Poster Presentation : **ORGN.P-149**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Azacyclohexanes and Acid-degradable cationic polyacrylates as siRNA Delivery vehicles

Seongjoo Park, Soo Kyung Cho*, Dai Il Jung, Jungtai Hahn¹

Department of Chemistry, Dong-A University, Korea

¹Department of Beauty Care, UI University, Korea

Studies on safe and effective drug delivery systems have been conducted steadily. Among them, Dendrimer is the best known drug delivery. However, increasing the molecular weight of these drug delivery vehicles can produce toxins in the body or cause unexpected side effects. In this study, a degradable 1,3,5-triazacyclohexane core synthesized from amino acids (Glycine, Valine, Cysteine, Serine, Aspartic acid, Glutamic acid, etc) reacted with degradable polyacrylates to form a fully degradable star polymers. High flexibility is expected from flexible core and star-shaped branches. Moreover, degradable core synthesized from amino acid and degradable ketal branches are expected to reduce the cytotoxicity as well. Spectroscopic characterization, polyplex morphology characterization as well as in vitro cytotoxicity and gene silencing efficiency will be discussed. Another study is to lead to the development of new medicines through the esterification of terminal hydroxyl groups of amino acids.

Poster Presentation : **ORGN.P-150**

Organic Chemistry

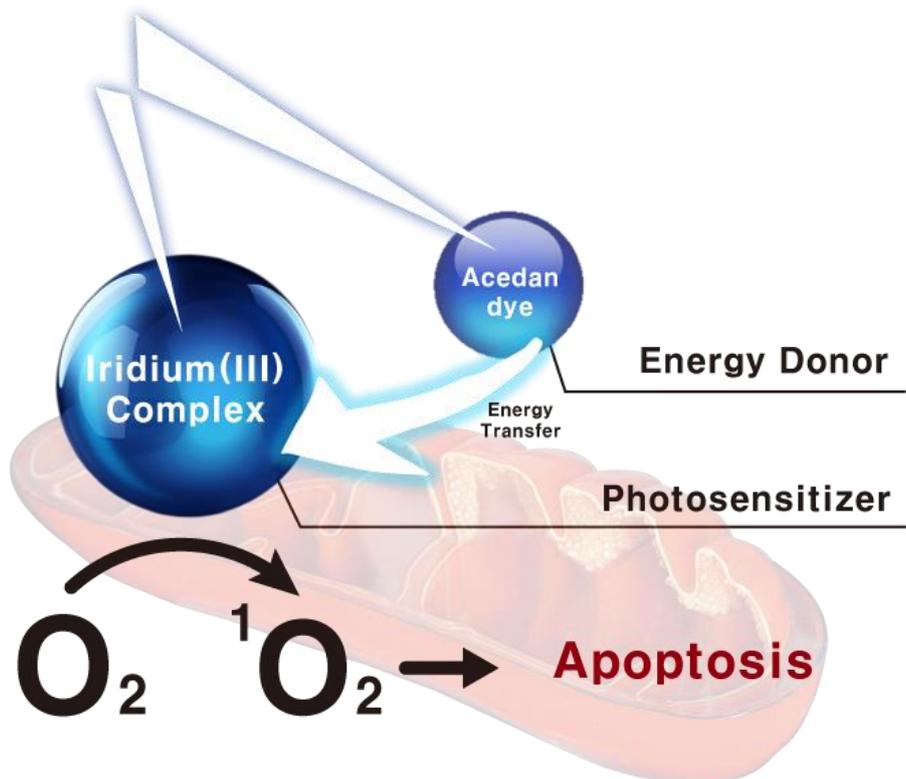
Grand Ballroom, THU 11:00~12:30

Enhancing ROS Generation via Photon Energy Transfer of Ir(III) Complex for Low Energy Photodynamic Therapy

Chaiheon Lee, Chae Gyu Lee, Tae-Hyuk Kwon*

Chemistry, Ulsan National Institute of Science and Technology, Korea

Ir(III) complexes with great reactive oxygen species (ROS) generation efficiency have attracted attention as photosensitizer for photodynamic therapy (PDT) because ROS such as singlet oxygen and superoxide radical induce protein inactivation and trigger cancer cell death. However, the Ir(III) complexes produce not enough amount of ROS to kill cancer cells due to low absorption coefficient despite their great ROS generation efficiency. Therefore, high-energy irradiation ($>35 \text{ J/cm}^2$) is necessary for PDT, which causes normal tissue damage in clinical application. Herein, we report novel Ir(III) complex, Ir-bxACD, incorporating acedan dye which has strong absorption coefficient, high quantum yield, and great two-photon activation property. As the Ir-bxACD is irradiated, the highly efficient intra-molecular energy transfer ($\geq 98\%$) occur because the emission energy of acedan dye is well-matched to absorption region of Ir(III) complex. Thereby, the enhanced amount of exciton of Ir-bxACD by energy transfer improves absolute amount of singlet oxygen. As a result, the Ir-bxACD with low-energy irradiation ($\leq 0.3 \text{ J/cm}^2$) triggers effective apoptosis on mitochondria of living cancer cells, even with two-photon activation. Consequently, we present rationally designed Ir(III) photosensitizer for PDT incorporating acedan dye, and propose the possibility of PDT using non-invasive irradiation.



Mitochondria in cancer cells

Poster Presentation : **ORGN.P-151**

Organic Chemistry

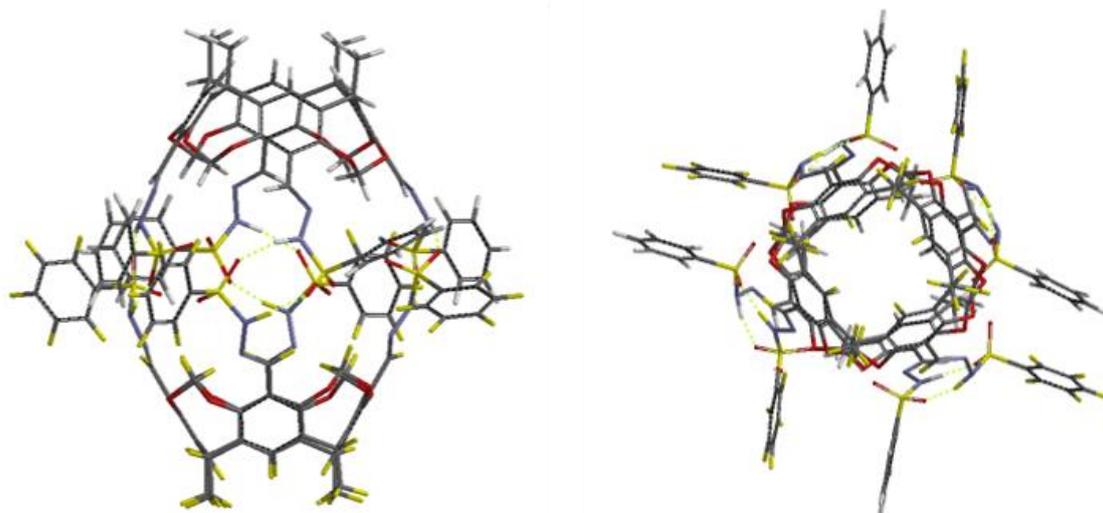
Grand Ballroom, THU 11:00~12:30

Resorcin[4]arene-Based sulfonamide molecular capsule

Yang ryeong Kim, Kyungsoo Paek*, Yeon Sil Park, Saegyo Jung

Department of Chemistry, Soongsil University, Korea

The self-assembled molecular capsules have been studied extensively due to their potentials as sensor, reaction chambers, and storage or deliver systems. A new self-assembled molecular capsule was designed and synthesized. The resorcin[4]arene-based sulfonamide cavitand formed stable molecular capsules in nonpolar solvents by the eight intermolecular N-H \cdots O=S hydrogen bonds in the presence of suitable guests. The synthesis and versatile characteristics of this sulfonamide molecular capsule toward various neutral or charged guests will be presented.



Poster Presentation : **ORGN.P-152**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Direct transamidation of secondary amide using Ni-catalyst: The role of TMSCl – Catalyst or Lewis Acid?

Subeen Yu, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Amides are ubiquitous in nature and are among the most essential molecules in the chemical and pharmaceutical industries. Transamidation is particularly useful, because it provides a direct and rapid means to diversify amides. However, the amide C-N linkage is unreactive due to resonance stabilization. Many studies have been reported using tertiary amide which have *N*-Boc, *N*-Ts scaffold. We studied nickel-catalyzed transamidation of secondary amide. We demonstrated that simple secondary amides such as *N*-phenylbenzamide and *N*-phenylcyclohexanecarboxamide were react with primary, secondary amine in the presence of nickel and TMSCl. In this reaction TMSCl is essential and it is shown good functional group tolerance.

Poster Presentation : **ORGN.P-153**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Palladium-Catalyzed C-S coupling & Carbonylation : Synthesis of *S*-Aryl thioesters

Myungjin Kim, Jieun Lee, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Thioesters were synthesized *via* palladium-catalyzed carbonylation of thioacetates and aryl iodides. *S*-Aryl thioacetates coupled with carbon monoxide and aryl iodides to afford the desired *S*-aryl thioesters in good yields. The reaction showed good functional group tolerance toward fluoro, chloro, ketone, ester, aldehyde, cyano, and nitro groups. The tandem reaction of the direct *S*-arylation of aryl iodides from potassium thioacetate (KSAc) and subsequent carbonylation of the intermediates *S*-aryl thioacetates provided *S*-aryl thioesters in moderate-to-good yields.

Poster Presentation : **ORGN.P-154**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of α,α -dihaloketone, α,α -dihalostilbene and 1,2-diketone from Alkyne and Dibromoisocyanuric acid

Eunjeong Cho, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

We developed sequential reaction of decarboxylative coupling and halogenation for the synthesis of α,α -dihaloketone. We accidentally confirmed that α,α -dihalostilbene and 1,2-diketone were formed. Previously, we reported the synthesis of 2,2-dichloro-1,2-diarylethanones from the reaction of diaryl alkyne and trichloroisocyanuric acid (TCCA). Only one example found a different product; α,α -dichlorostilbene. To expand our studies, we tried to employ dibromoisocyanuric acid (DBCA) as brominating reagent. We found that α,α -dibromostilbene and 1,2-diketone were synthesized at the same time. We tried to control appropriate condition to get 1,2-diketone predominantly. Mostly, Synthesis of 1,2-diketone is performed in the presence of Metal. Because of Metal Free, our studies have some advantages and we hope to contribute new process.

Poster Presentation : **ORGN.P-155**

Organic Chemistry

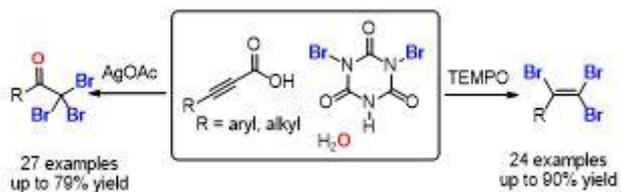
Grand Ballroom, THU 11:00~12:30

Selective Synthesis of Tribromomethyl Ketone and Tribromovinyl derivatives: The Role of AgOAc and TEMPO

Aravindan Jayaraman, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Tribromomethyl ketone and tribromovinyl derivatives were selectively prepared from the decarboxylative tribromination. The reaction between propiolic acid derivatives and dibromoisocyanuric acid (DBCA)/H₂O afforded predominantly a tribromomethyl ketone derivative in the presence of AgOAc (10 mol%). When the same reaction was conducted with 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) instead of AgOAc, tribromovinyl derivatives were exclusively formed in good yields. It was found that ethynyl bromide is an intermediate.



Poster Presentation : **ORGN.P-156**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Highly regio-selective radiofluorination of 2,4,6-trimethoxyphenyl(aryl)iodonium salts to produce electron-rich [¹⁸F]fluoroarenes

Young-Do Kwon, Jeongmin Son¹, Joong-Hyun Chun*

Department of Nuclear Medicine, Yonsei University College of Medicine, Korea

¹Department of Nuclear Medicine, Severance Hospital, Korea

Due to expanding interest in the development of fluorine-18 labeled radiopharmaceuticals in molecular imaging with positron emission tomography (PET), regio-selective incorporation of fluorine-18 ($t_{1/2} = 109.7$ min) onto electron-rich aryl rings is particularly required. Reaction of [¹⁸F]fluoride ion with diaryliodonium salt has been known for an efficient method for single-step introduction of fluorine-18 into aromatic substrates; however, diaryliodonium salts ($\text{ArI}^+\text{Ar}'\text{X}^-$) react with [¹⁸F]fluoride ion to give $\text{Ar-}^{18}\text{F}$ and $\text{Ar}'\text{-}^{18}\text{F}$ as radio-fluorinated products. Numerous efforts have been made to improve selectivity between the two resulting aryl rings. Herein, we introduce the 2,4,6-trimethoxyphenyl (TMP)-derived iodonium tosylates as precursors for [¹⁸F]fluoroarenes with high ring selectivity. The dried [¹⁸F]fluoride ion complex and iodonium salt precursor were reacted at 120–160 °C, and the radiofluorinated products were analyzed using radio-HPLC to determine radiochemical yields (RCYs). The selectivity for $\text{Ar-}^{18}\text{F}$ vs. ^{18}F -2,4,6-trimethoxybenzene was determined for each reaction. Electron-rich aryl rings, such as 2-anisole, mesitylene, and biphenyl, were radiofluorinated in a highly selective manner to yield the corresponding [¹⁸F]fluoroarenes in 3–77% RCYs. Given that the TMP-derived iodonium salts showed a remarkable selectivity for electron-rich [¹⁸F]aryl fluorides in useful RCYs, the application of this methodology could afford efficient and reliable preparative routes to potential aromatic PET radioradiotracers. This work was funded by the National Research Foundation (NRF-2015R1D1A1A02061420) of Korea.

Poster Presentation : **ORGN.P-157**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Development of novel carbapenem-based fluorogenic probe for specific detection of carbapenemase-producing organisms

Juhyeon Kim, Hyunah Choo¹, Hak Joong Kim, Sun-Joon Min^{2,*}

Department of Chemistry, Korea University, Korea

¹*Center for Neuro-Medicine, Korea Institute of Science and Technology, Korea*

²*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

The emergence and rapid spread of antibiotic resistant bacteria is becoming a major public health crisis worldwide. In particular, the resistance against β -lactam antibiotics is currently increasing at an alarming rate. Carbapenem, which is called the antibiotic of the last resort, is very effective in treating bacterial infections due to its broad activity against bacterial pathogens and excellent stability against most β -lactamases. However, carbapenem resistant bacteria have also been frequently observed in recent years with extensive use of carbapenem antibiotics. The major mechanism of resistance to carbapenem in bacterial pathogen is related to the expression of carbapenemase that hydrolyzes almost all antibiotics with the β -lactam ring. Up to date, about 20 types of carbapenemases have been reported including KPC (Ambler class A), VIM, IMP, NDM (Ambler class B), and OXA (Ambler class D). Because each type of carbapenemases shows different tolerance to a certain carbapenem, there is a great difficulty in detecting the carbapenemase-producing organisms (CPOs) with a simple detection method. Therefore, efficient and accurate detection of CPOs is critically important for rigorous infection control and therapeutic guidance. There are several methods for the detection of CPOs, such as the Modified Hodge test (MHT), Carba NP test and Polymerase chain reaction (PCR) based methods. Most of the current methods lack specificity and sensitivity and are time-consuming (e.g., MHT, carba NP) or require expensive instruments and high cost (e.g., PCR based methods). A number of studies have been conducted to overcome these disadvantages, among which the fluorescence-based detection methods have become attractive due to their high sensitivity, low costs, and operational simplicity. In this study, we have developed a series of fluorescence substrates with a carbapenem core structure for the specific detection of carbapenemase in CPOs. This fluorogenic probes exhibit enhancement of fluorescence intensity upon hydrolysis by carbapenemase. In addition, clinical experiments have demonstrated that the new probes have the potential

to rapidly and accurately detect carbapenem-expressing organisms for timely diagnosis and treatment of infected patients.

Poster Presentation : **ORGN.P-158**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

The synthesis of benzoxazole compounds and their anticancer activities

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Benzoxazole compounds, 2-aryl substituted benzene-fused oxazole ring structure, were one of the most important class of heterocyclic scaffold exhibiting remarkable biological properties including antibacterial, antifungal, anti-inflammatory, antiviral, anticancer, analgesic, anticonvulsant, antioxidant, antidepressant, anthelmintic, and herbicidal. Recently, seven new benzoxazole derivatives, nocarbenzoxazoles A-G, were isolated from *Nocardioopsis lucentensis* DSM 44048. The isolated compounds showed selective anticancer activity against HepG2 and HeLa. During the research for developing various pharmaceutical compounds, we were able to develop a facile synthetic method for benzoxazole derivatives using 2-H benzoxazole intermediate. Eight new benzoxazoles could be efficiently obtained. It showed selective anticancer activity against HeLa cell line(uterine cervical cancel).

Poster Presentation : **ORGN.P-159**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

The Mechanistic Study of Alkyne Arylation via Nucleopalladation

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

In recent decades, the alkyne-directed transformations catalyzed by palladium have become a powerful tool to construct highly functionalized products. Hydroamination is an attractive and easy strategy to functionalize alkynes, where we can utilize the both Markovnikov and anti-Markovnikov variations that result in regioselectivity.¹ In this case, regioselectivity for aminopalladation step depends on the amine attack used as a directing group for C-C bond formation.

To date, only one intermolecular, two component aminoarylation has been demonstrated.² Here, we hypothesized, aryl triflate, amine and alkyne-based three component regioselective reaction results vinylpalladium(II)-intermediate that upon hydrolysis give either α,α -diarylketone or α -arylphenone. The choice of amine controls the regioselectivity via nucleopalladation step, where the bulky amine favor to attack less hindered terminal of alkyne substrate. For computational simplicity, we used DPPF and Mandyphos-based model ligands for Pd (0) catalyst and a possible reaction mechanism for C-H activation is proposed.³

References

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Poster Presentation : **ORGN.P-160**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Study of synthesis of 9,9',13,13'-tetra-Phenyl-substituted-carotenoids.

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Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Phenyl substituents attached to the polyene chain provide not only improved stability, but also diverse physicochemical characteristics, depending on the electronic nature of the substituent. Carotene with tetra-Phenyl substituents has better electrical conductivity than carotene with di-Phenyl substituents. Carotenoid molecular wires containing tetra-Phenyl substituents can be assembled by the Wittig reaction between tetra-Phenyl-substituted-dial and 4-thiomethylbenzyl phosphonium bromide(Wittig salt). tetra-Phenyl-substitued-dial can be more effectively synthesized by the Julia-Kocienski olefination of the Phenyl-substituted-C5-BT(benzothiazole)-sulfone with C10 2,7-diphenyl-2,4,6-octatrienedial than double elimination.

Poster Presentation : **ORGN.P-161**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Efficient synthesis from D-glucose to Pyrrolo-lactone compound

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Department of Energy science and Technology, Myungji University, Korea

¹Department of Chemistry, Myungji University, Korea

5-(Hydroxymethyl)-2-furfural(5-HMF) is well known as the next generation platform chemical in biomass industry. We tried to obtain 5-HMF using primary amine and D-glucose through N-glycosylation, Amadori reaction and Mailard reaction. We have added an amino ester to assist the ring opening and rearrangement of D-glucose. As a result, Sedative and antiinflammatory pyrrolo-lactone compounds were obtained which can be extracted from natural plant as folk medicine.

Poster Presentation : **ORGN.P-162**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthetic method of diversely R-substituted 4-hydroxybenzoic esters - Oxidation of substituted Hagemann's ester

Dahye Kim, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

In an effort to synthesize carotenoids with improved biological activity, we need to develop a practical synthetic method of diversely R-substituted 4-hydroxybenzoic esters as the terminal ring structure. A practical two-step synthetic method of diversely R-substituted 4-hydroxybenzoic esters, which may have wide applications in household chemicals and polymeric materials, was developed by 2:1 coupling between ethyl acetoacetate and aldehydes (RCHO) in t-BuOK/t-BuOH, followed by oxidative aromatization of the resulting Hagemann's esters by using stoichiometric NBS and catalytic TMS.OTf.

Poster Presentation : **ORGN.P-163**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Research of synthetic method of Unnatural carotenoids

Bo-ram Lim, Sangho Koo*

Department of Chemistry, Myungji University, Korea

Unnatural carotenoids containing various phenyl substituents has excellent characteristic in terms of stability and electronic conductance. We have developed a series of efficient synthetic methods of natural carotenoids, that can be further extended to the synthesis of the unnatural stabilized carotenoids as a molecular wire. So, It is necessary to design efficient building blocks ; Under the sequence of Indium mediated addition and Oxonia-cope rearrangement reaction, allylic sulfone unit containing aromatic substituents can be readily prepared from Acetophenone derivatives. And dialdehyde unit could be easily onbtained. The unnatural carotenoids can be synthesized by the coupling reaction between allylic sulfone unit and dialdehyde unit , Protecting reaction and double elimination reaction. Therefore, we were able to measure electrical conductivity using unnatural carotenoid wires.

Poster Presentation : **ORGN.P-164**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

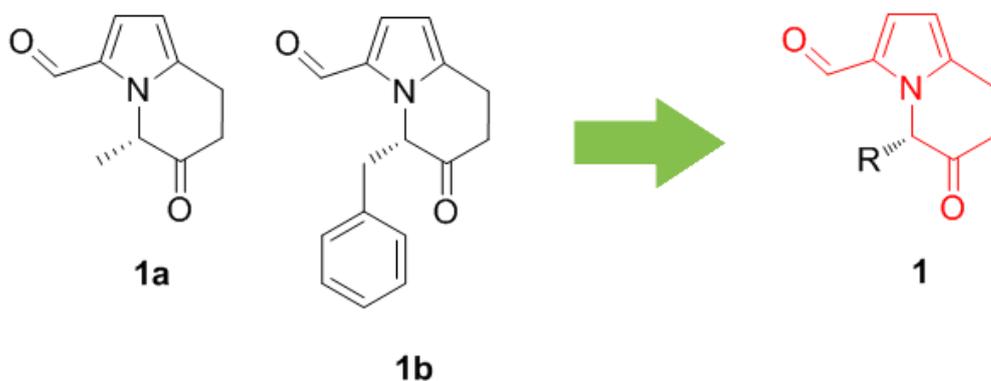
One-pot Synthetic methods of Pyrrolo Lactone compound

Ik Joon In, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

The compounds 1a and 1b are the key components of traditional folk medicine extracted from *Celastrus orbiculatus* and *Capparis spinosa* respectively. The Maillard reaction between amino acid and sugar produces various volatile products. The Maillard reaction produces very little amount of pyrrole form [1]. We developed a mild Maillard variant, which reacted sugar and amino acid in oxalic acid and DMSO at 65~90°C to give 30~40% yield of pyrrolo lacton 1. This reaction can make various amino acids and sugars easily and practically for 1 form. Diversely R-substituted pyrrolo lactone 1 can be obtained depending on the form of amino acid. It is expected that this pyrrolo lactone compound can possibly be the next generation of analgesic drugs, human-friendly seasonings and functional materials.



Poster Presentation : **ORGN.P-165**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Adaptation of High Throughput Screening in Novel Antioxidant Discovery

Gaosheng Shi, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myongji University, China

¹Department of Chemistry, Myungji University, Korea

High throughput screening, which is widely applied in biochemical science, is one of the new and effective approaches to the drug discovery. High throughput has been implemented to the automation of robots, detectors and software. We applied this method to screening the antioxidant activity of novel carotenoids, adding the statistics of the algorithm (cluster analysis and principal component analysis), which can establish a new model to analyze the structure-activity relationship of carotenoid derivatives and screen target antioxidant in a short time.

Poster Presentation : **ORGN.P-166**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

The application of Mn(III)/Co(II) Catalyzed Oxidative Deacetylation In Important Heterocyclic Compounds Synthesis

Hui Jin, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, China

¹*Department of Chemistry, Myungji University, Korea*

The conjugate addition of 1,3-dicarbonyl compounds to α , β -unsaturated carbonyl compounds produce 1,5-dicarbonyl compounds, which are ideally suited for the Mn(III)/Co(II)-catalyzed oxidative deacetylation to form 1,4-dicarbonyl compounds. A new type of hetero-cyclization directed by a 1,4-dicarbonyl compound has been developed. Based on the above oxidation, a high yield of oxidative deacetylation was gained under the condition of 5 mol% Mn(AcO)₃ and 2 mol% CoCl₂. One pot syntheses of furan, thiophene, and pyrrole were accomplished by using Mn(III)/Co(II) catalytic oxidative deacetylation. Further work on extending this catalytic oxidative reaction to the synthesis of some natural products is ongoing.

Poster Presentation : **ORGN.P-167**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Polyphenols Using an Efficient Deprotection of Benzenesulfonyl Protection

Mohammad Shariful Alam, Sangho Koo^{1,*}

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¹Department of Chemistry, Myungji University, Korea

A robust repertoire for phenol protection/deprotection was demonstrated by the use of durable benzenesulfonyl group, which survives many harsh reaction conditions using Grignard reagents, organolithium reagents, metal alkoxides, phosgenes, mineral and Lewis acids etc. A facile deprotection condition utilizing pulverized KOH and t-BuOH in hot toluene make this protocol as a practical method which can be applied to the multi-step synthesis of biologically and medicinally important polyphenol compounds.

Poster Presentation : **ORGN.P-168**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

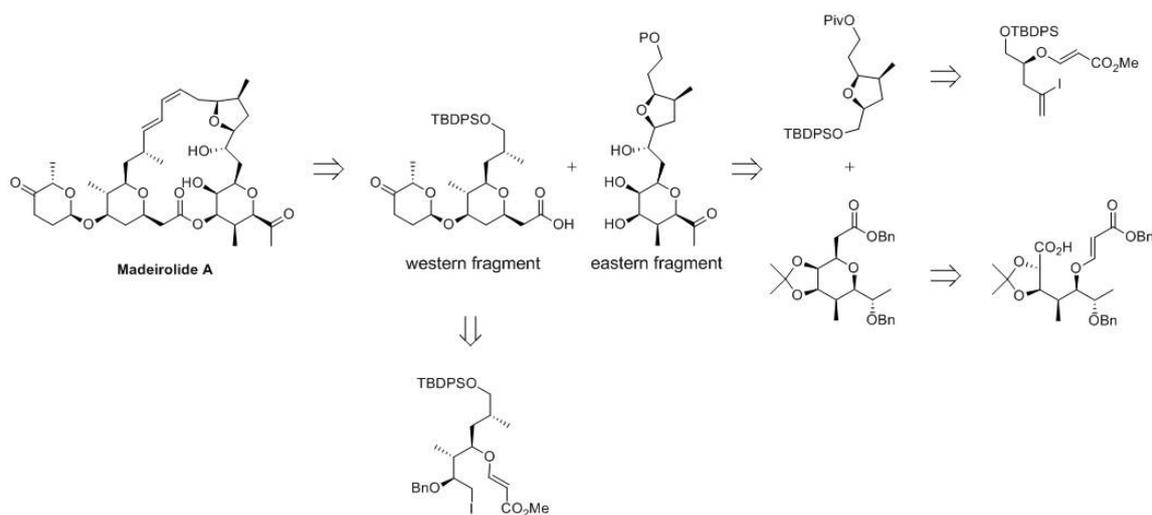
Synthetic Studies toward Madeirolide A

Wookyong Eo, Chulbom Lee^{1,*}

Department of Chemistry, Seoul National University, Korea

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

Madeirolide A is a marine macrolide, isolated from a marine sponge of the *Leiodermatium* species off the coast of Porto Santo, Portugal, by Wright and Winder in 2009. This natural product exhibits potent inhibitory effects in the fungal pathogen, *Candida albicans*, on a microgram scale (12.5 $\mu\text{g/mL}$). The chemical synthesis of madeirolide A is highly desirable, due to the difficulty associated with its isolation, as well as its intriguing structure. Madeirolide A is a 24-membered macrolactone, possessing 16 stereogenic centers, an *E,Z*-diene and three *cis*-oxacycle moieties. Three partial syntheses have been reported for the western fragment – a 2,6-*cis*-THP ring with a glycosidic linkage – wherein the synthetic strategies have focused on the construction of the 2,6-*cis*-THP ring. Here, we present our efforts towards a convergent and enantioselective synthesis of madeirolide A. Three oxacyclic subunits, which can be assembled to form madeirolide A, have been synthesized from β -alkoxyacrylates using visible-light-induced photocatalytic radical cyclizations. The assembly of three subunits is ongoing now.



Poster Presentation : **ORGN.P-169**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Luminescence Behavior of Bent Shaped Organic Nanoparticles Based on Excited State Intramolecular Proton Transfer

Mithun Santra, Ye Jin Reo¹, Kyo Han Ahn^{1,*}

The University of Edinburgh, United Kingdom

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

Fluorogenic materials that emit both in solution and in solid states have received special attention for their potential applicability to optoelectronic devices and biochemical sensing systems.¹ In order to explore the molecular shape dependent luminescence, we synthesized bent shaped 1-(benzo[d]thiazol-2-yl)-6-substituted-naphthalen-2-ol (BTN) compounds and their 2-methoxy derivatives and found out that they show luminescence both in solution and in solid states, plausibly due to unfavorable orbital interactions between stacked molecules.² The naphthol compounds also showed large Stokes shifts due to the ESIPT feature, along with good optical brightness and tunable emission color by changing the 6-substituent. Photophysical properties of the new dyes and their nanoparticles in solution and solid states (in powder and crystalline forms) were characterized by spectral analysis and fluorescence lifetime measurements. The new organic nanoparticles were shown to stain cells by both confocal and two-photon microscopic imaging. The approach of molecular shape control demonstrated here thus opens a door toward solid-state luminescent organic compounds and their nanoparticles. References [1] An, B. K. Ahn, S. K. Kwon, S. D. Jung, S. Y. Park, J. Am. Chem. Soc. 2002, 124, 14410. [2] M. Santra, Y. W. Jun, Y. J. Reo, S. Sarkar, W. Choi, J. E. Kwon, S. Y. Park, K. H. Ahn, ACS Appl. Bio. Mater. 2018, 1, 136.

Poster Presentation : **ORGN.P-170**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Chiral Lewis Base-Catalyzed Kinetic Resolution of α,α -Dihalo-*cis*-vinyl Epoxide

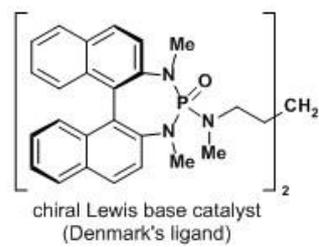
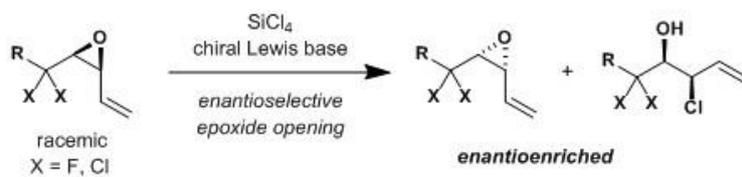
Jungi Jung, Jae Hee Kim, Won-jin Chung*

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

Vinyl epoxides are versatile precursors to highly functionalized compounds.¹ The combination of olefin and epoxide affords not only unique reactivity that cannot be harnessed from each moiety alone but also effective properties of the two functional groups. Because of the high utility of vinyl epoxide, various synthetic methods and strategies have been studied and applied to total synthesis of natural products. Nevertheless, enantioselective synthesis of vinyl epoxide is challenging and typically depends on enantioselective epoxidations of a few types of substrate. Kinetic resolution can be employed as an alternative strategy when no general, enantioselective synthetic method is available. Kinetic resolution has been successfully utilized for the synthesis of highly enantioenriched vinyl epoxide intermediates in total syntheses of chlorosulfolipids.² Because Denmark's catalyst had provided good selectivity in kinetic resolution of dichlorinated α,β -*cis*-vinyl epoxide, other types of substrates including α,α -dihalogenated epoxides are examined under Denmark's Lewis base-catalyzed enantioselective chlorinolysis conditions.³

References

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2. (a) Chung, W.-j.; Carlson, J. S.; Vanderwal, C. D. *J. Org. Chem.* **2014**, *79*, 2226–2241. (b) Chung, W.-j.; Carlson, J. S.; Bedke, D. K.; Vanderwal, C. D. *Angew. Chem. Int. Ed.* **2013**, *52*, 10052–10055.
3. (a) Denmark, S. E.; Barsanti, P. A.; Beutner, G. L.; Wilson, T. W. *Adv. Synth. Catal.* **2007**, *349*, 567–582. (b) Denmark, S. E.; Barsnati, P. A.; Wong, K.-T.; Stavenger, R. A. *J. Org. Chem.* **1998**, *8*, 2428–2429.



Poster Presentation : **ORGN.P-171**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Selective Alkenylation of *N*-alkylpyrroles Using Electronically Complementing Ligand Systems.

HyunTae Kim, Woohyeong Lee, Eunmin Kim, Jung Min Joo*

Department of Chemistry, Pusan National University, Korea

Pyrroles are important targets for C-H functionalization because of their prevalence in polymers, dyes, and drugs, including atorvastatin, ketorolac, and tolmetin. However, C-H functionalization of the parent pyrroles presents challenges in achieving regioselectivity and preventing polymerization of the pyrroles under acidic and oxidative conditions. We developed an undirected, aerobic strategy for the C-H alkenylation of *N*-alkylpyrroles by ligand control. For C2-alkenylation of electron-rich *N*-alkylpyrroles, an electrophilic palladium catalyst derived from Pd(OAc)₂ and 4,5-diazafluoren-9-one (DAF) was used. Alternatively, a combination of Pd(OAc)₂ and a mono-protected amino acid ligand, Ac-Val-OH, was useful for C5-alkenylation of *N*-alkylpyrroles possessing electron-withdrawing groups at the C2 position.

Poster Presentation : **ORGN.P-172**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Atom economic synthesis and characterization of ionic liquids with bis(trifluoromethanesulfonyl)imide as anion

Seong Yeol Lee^{*}, Eul Kgun Yum, Gi Hyeon Sung¹, Jiho Yoo¹, Youngjin Jeong¹

Department of Chemistry, Chungnam National University, Korea

¹Annex Research Institute, Sejong Chemical Co., Ltd, Korea

Tributylmethylammonium bis(trifluoromethanesulfonyl)imide (TBMA-TFSI), an ionic liquid, is widely used as an antistatic agent for polarizing films. Herein, TBMA-TFSI was synthesized by atom-economic butylation from dibutylmethylamine (DBMA) using bis(trifluoromethanesulfonyl)imide (*N*-Bu-TFSI) as a key intermediate. This synthetic method was applied to 1-methylimidazole and 1-methylpyrrolidine, leading to synthesis of ionic liquids (1-butyl-3-methylimidazolium)-TFSI and (1-butyl methyl pyrrolidinium)-TFSI with very good yields. Physical and chemical properties of these prepared ionic liquids were then characterized for applications as antistatic agents and electrolytes.

Poster Presentation : **ORGN.P-173**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Study on TG-DSC and ionic conductivity according to spacer structure of imidazolium-based poly(ionic liquid)s

Seong Yeol Lee^{*}, Eul Kgun Yum, Gi Hyeon Sung¹, Jiho Yoo¹, Youngjin Jeong¹

Department of Chemistry, Chungnam National University, Korea

¹Annex Research Institute, Sejong Chemical Co., Korea

Poly(ionic liquid)s (PILs) were synthesized by grafting alkyl and ethylene glycol onto poly vinylimidazole having the same degree of polymerization. Furthermore, poly(1-vinyl-3-substituted-imidazolium TFSI) was synthesized via the ion exchange of counter anions with bis(trifluoromethanesulfonyl)imide (TFSI). These PILs were analyzed using differential scanning calorimetry and thermogravimetric analysis, and a comparative analysis was performed for properties of glass transition temperature (T_g) and ionic conductivity according to the substituent change of PILs through impedance measurements.

Poster Presentation : **ORGN.P-174**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Anion Binding of an Indolocarbazole-Pyridine Foldamer via a Site-specific Chemical Modification

Hyemi Lee, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

Recently, many efforts have been devoted to utilize artificial foldamers as receptors for biologically important guests. Previously, we synthesized a series of indolocarbazole-pyridine (IP) hybrid foldamers that adopted helical conformations in solution and solid state. Upon helical folding, the IP foldamers were found to produce an internal cavity wherein three to four water molecules were tightly occupied by multiple hydrogen bonds. These hydrogen bonds prevent the IP foldamers functioning as a synthetic receptor. With this in mind, we have synthesized a new IP heptamer containing an inverted pyridine unit in the middle of the strand, so that the CH of the pyridine directs to the internal cavity to weaken the hydrogen-bonding network. As a result, this heptamer enables to encapsulate two of dihydrogen phosphates as a dimeric form as characterized by ^1H NMR, UV-vis spectroscopy, ITC titrations and X-ray single crystal structures. All the details including will be described in the presentation.

Poster Presentation : **ORGN.P-175**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and characterization of benzotriazole derivatives for UV absorber

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Research Center for Green Fine Chemicals, Korea Research Institute of Chemical Technology, Korea

¹*Convergent Chemistry Division, Korea Research Institute of Chemical Technology, Korea*

²*Department of Chemistry, Pusan National University, Korea*

Ultraviolet rays from the sun are composed of UVA, UVB, and UVC. But only UVA and UVB are reaching on the surface while UVC is completely filtered by the atmosphere. UVB is a cause of skin aging, stinging, burns, etc. UVA has little effect on human body but seriously damages rubber, plastic, fiber, building outer wall, paint and change the physical properties. It is a common industrial practice to use UVA absorbers as an additives to prevent damage caused by UVA. In this study, uv absorbance, heat stability, and color of solution characteristics were investigated by varying the alkyl group of benzotriazole UVA absorbers with the highest ultraviolet absorption in the UVA region. The colors of synthesized benzotriazole derivatives were refined using thin film short path to improve the color of solution. Among the synthesized benzotriazole derivatives, benzotriazole ultraviolet absorber with linear alkyl group showed the best UV absorption and thermal stability.

Poster Presentation : **ORGN.P-176**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Copper-Catalyzed 1,2-Bis(trifluoromethylation) of Alkenes

Hyunseok Oh, AReum Park, Soo Bong Han^{1,*}, Kyu-Sung Jeong^{*}, Hyuk Lee^{1,*}

Department of Chemistry, Yonsei University, Korea

¹Innovative Therapeutics Research Center, Korea Research Institute of Chemical Technology, Korea

Trifluoromethyl group (CF₃) has attracted in various research fields because of its ability to improve the lipophilicity, metabolic stability, and bioavailability of many compounds. CF₃ is usually a key structural component of many biologically active compounds in pharmaceuticals and agrochemicals. 1,2-Difunctionalization of alkenes is one of the most useful methods to synthesize more complex and multi-functionalized molecules. In this study, CF₃ was introduced by 1,2-difunctionalization of alkenes to prepare 1,2-bistrifluoromethylated compounds. Various compounds with CF₃ was successfully synthesized by optimized conditions with a copper catalyst. Mechanism would be investigated through further study.

Poster Presentation : **ORGN.P-177**

Organic Chemistry

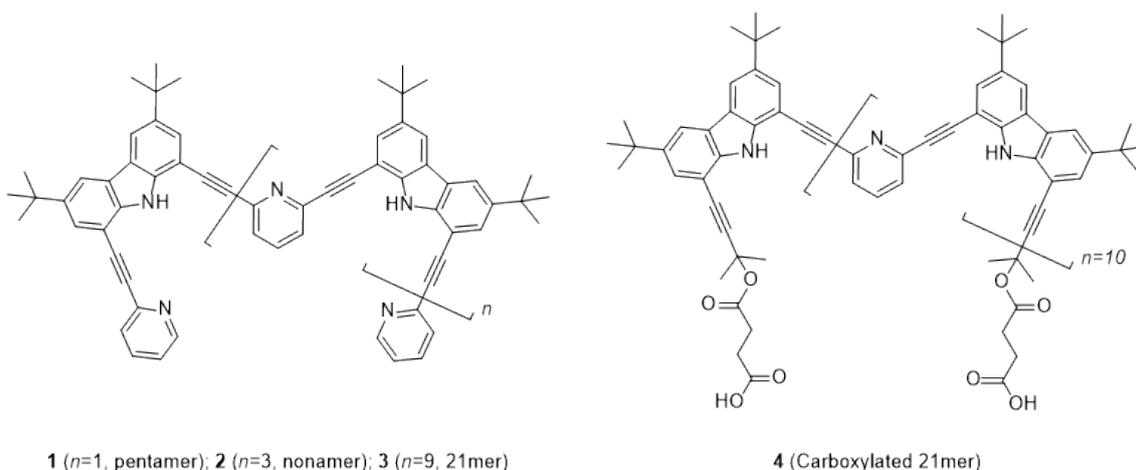
Grand Ballroom, THU 11:00~12:30

Carbazole-Pyridine Foldamers Capable of Functioning as a Synthetic Transmembrane Channel

ByungJun An, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

The movement of various ions and water in cell membranes have a crucial role in human body. To understand the underlying principles and mechanisms of transmembrane channels, many transport molecules were designed over the past few decades. Especially unimolecular transmembrane channels were designed and prepared in supramolecular chemistry. Herein, we have designed a series of aromatic foldamers 1-3 that consist of two different repeating monomers, carbazole and pyridine, which are connected through ethynyl bond. The lengths of internal voids are varied up to a few nanometers, thus the foldamers possibly functioning as a unimolecular transmembrane channel. Especially, foldamer 4 contains carboxylate groups at both ends for anchoring in an aqueous phase. Details including syntheses and folding behaviours will be discussed in the presentation.



Poster Presentation : **ORGN.P-178**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Design, Synthesis and Evaluation of Amino Benzyne Precursors Triggered by 1,3-Aza-Brook Rearrangement

Young-Kyo Jeon, Yeseul Yun¹, Kyeong Eun Kim², Wonsuk Kim^{2,*}

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

¹*Ewha Womans University, Korea*

²*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Considering the recent advances in benzyne chemistry, amino-substituted benzyne could be used for promising synthetic tools in preparation of diverse aniline derivatives. Currently, amino-substituted ortho-silylaryl triflates are common amino benzyne precursors which are induced by a fluoride source. However, only a few studies on amino benzyne species and their applications have still been reported. Thus, herein, we report the design, synthesis and evaluation of new type of amino benzyne precursors which can generate amino benzyne intermediate triggered by 1,3-aza-brook rearrangement. Furthermore, we present the highly regioselective reactions between various arynophiles and amino- benzyne generated from 3-amino benzyne precursor and whether DFT calculations are effective at rationalizing the observed selectivities.

Poster Presentation : **ORGN.P-179**

Organic Chemistry

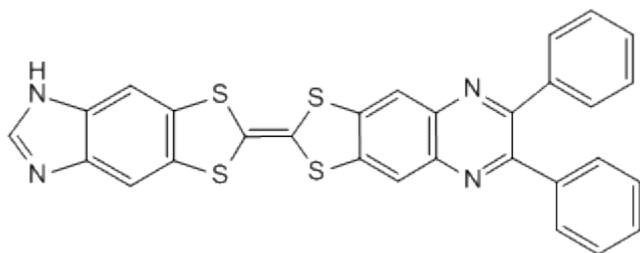
Grand Ballroom, THU 11:00~12:30

Step-wise Protonation Controlable Electrochemical and Photochemical Properties in Quinoxaline-tetrathiafulvalene-imidazoles

Trang Thu Tran, Ngan Nguyen, Jung Su Park*

Department of Chemistry, Sookmyung Women's University, Korea

Fused electron donor-acceptor (D-A) systems have been attracted intensive research during the past few decades due to their potential applications, including in creating the low-banding gap systems, artificial photosynthetic systems, molecular electronics. We report here the synthesis and characterization of imidazole fused tetrathiafulvalene derivatives. These materials exhibit intramolecular electron-transfer and leads to formation of diradical states. Upon the protonation, largely red-shifted ICT band were observed. Furthermore, the protonated derivatives show amphoteric redox behavior and charge-separated diradical character. The molecular structures were fully characterized by NMR, Mass-spectroscopic as well as X-ray crystallographic studies. The electrochemical and photophysical properties of these derivatives will be discussed in details based on UV-Vis, Fluorescence, EPR, Cyclic Voltammetric and Differential Pulse Voltammetric studies.



Poster Presentation : **ORGN.P-180**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Dicationic *N*-Alkylpyrrolidinium Salts Organic Ionic Plastic Crystals

Hyun Ho Chae, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

A series of bis-pyrrolidinium salts have been synthesized as new organic ionic plastic crystals (OIPCs). The most C₂ and C₄ alkylene bridged bis-pyrrolidinium Br⁻, I⁻, PF₆⁻, Tf₂N⁻ salts show solid-solid phase transitions. Thermal gravimetric analysis show their thermal stabilities; halide salts are less stable than PF₆ or Tf₂N salts. 1,2-Bis[*N*-(*N*-dodecylpyrrolidinium)]ethane 2I⁻ (T_{ss} = 18 °C, T_m = 158 °C) show a entropy of fusion, ΔS_f = 9 J mol⁻¹ K⁻¹, which satisfies value of Timmermans' definition of plastic crystals (ΔS_f = 20 J mol⁻¹ K⁻¹). Multiple solid phase transitions, structure of the compounds and ionic conductivity studies through a temperature change are investigated.

Poster Presentation : **ORGN.P-181**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of 2-Naphthol Derivatives through Metal-Free C(sp²)-H Bond Insertion Reaction Using α -Diazocarbonyl Compounds

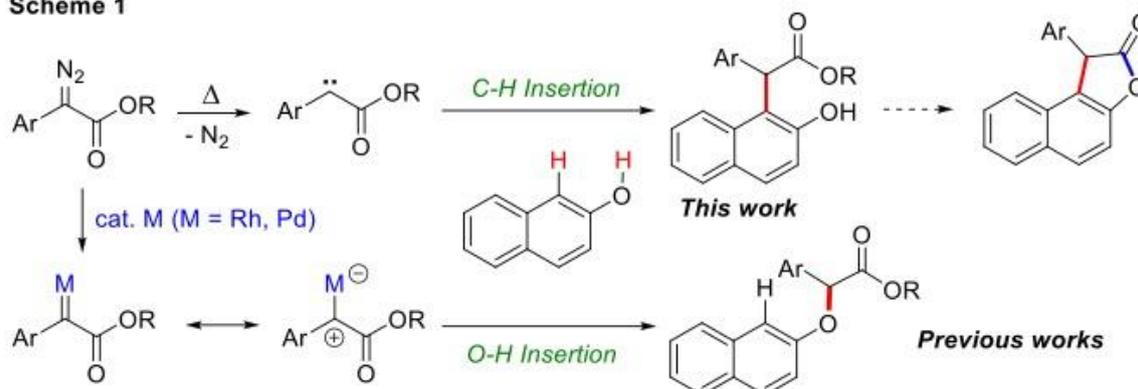
Dajung Jung, Jiwon Kim, Sang-gi Lee^{1,*}

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

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

Diazo compounds, as precursors of reactive metal carbenoids, have been overwhelmingly utilized for the development of versatile synthetic methods in modern organic synthesis. For examples, donor/acceptor metal-carbenoids possessing tractable electrophilic reactivity have been used in various transformations including cyclopropanations, X-H bond (X= O, N, C, S) insertions, and ylide formations. Meanwhile, controlling reactivity of donor/acceptor carbenes toward O-H or C-H bond insertions of phenol derivatives has been considered as one of the challenging issues. In recent studies, it has been demonstrated that in the presence of Au and boron catalysts, the α -diazooesters could undergo the chemoselective and sitespecific C-H bond substitution into the phenols. In present work, to our surprise, we found that thermally induced less controllable metal-free carbenes are introduced into β -naphthol exclusively via α -C(sp²)-H bond insertion to afford 2-naphthol-substituted carboxylates, which can be readily transformed into naphtho[2,1-b]furan-2(1H)-ones, pharmaceutically useful bioactive frameworks.

Scheme 1



Poster Presentation : **ORGN.P-182**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Dicationic *N*-Alkylpiperidinium Salts Organic Ionic Plastic Crystals

JongChan Shin, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

A series of bis-alkylpiperidinium salts have been synthesized as new organic ionic plastic crystals (OIPCs). Ethylene bridged bis-piperidinium salts are synthesized with n-dodecyl and n-decyl alkyl chains. Butylene bridged bis-piperidinium are with n-heptyl, n-octyl, n-decyl. All bis-piperidiniums are synthesized as Br salts first and then anion exchange reactions give corresponding I⁻, PF₆⁻, and Tf₂N⁻ compounds. Thermal gravimetric analysis show their thermal stabilities; halide salts are less stable than PF₆ or Tf₂N salts. Multiple solid phase transitions, structure of the compounds and ionic conductivity studies through a temperature change are investigated.

Poster Presentation : **ORGN.P-183**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

s-Triazine Based Oxidized Carbon Nitride : Directly Gd Chelatable Nanoparticle for MR Imaging

Chul Hee Kim, Dong Wook Kim*

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Gd-based contrast-agents(CAs) are used as one of the powerful tools for diagnosing various diseases in modern magnetic resonance imaging (MRI). MR images are acquired by signal from water in each organs and strongly relied on that of T1 relaxation time. By shortening T1 relaxation time of surrounding water, Gd-based CAs enhance the signal and notify us information of lesions. Nevertheless, The use of Gd-CAs in human body are restrictively allowed because of low r1 value derived from some Gd-chelators and absence of targeting properties toward lesions. Here we suggest directly Gd-chelatable nanoparticle, oxidized carbon nitride (OCN). OCN was synthesized by top-down method via treating oxidant to s-triazine based carbon nitride and demonstrated its properties through many analytical instruments. OCN showed its high Gd³⁺-chelatable nature and targeting ability toward tumor by experiment on animals.

Poster Presentation : **ORGN.P-184**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

One-pot Construction of Heterocycles having Quaternary Carbon Center via Dual Rh(II)/Pd(0) Relay Catalysis

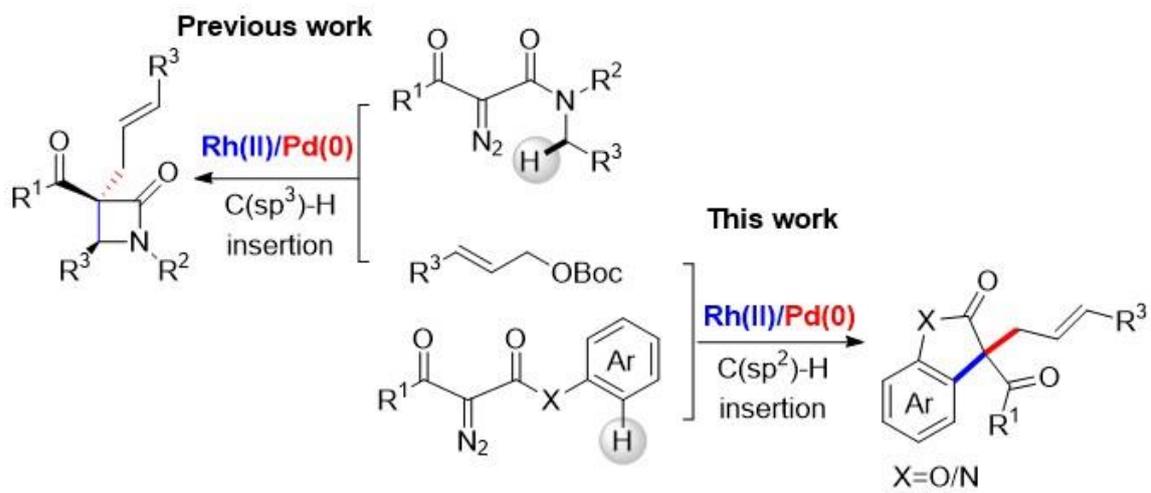
Zi Xuan , Yu lim Lee¹, Sang-gi Lee^{2,*}

Chemistry Department of Nano, Ewha Womans University, Korea

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²*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Heterocyclic compounds having a quaternary carbon center are frequently found in a range of natural products and bioactive molecules. Accordingly, the development of an efficient and environmentally benign synthetic methods is highly desirable. In this regards, dual relay catalysis is considered as one of the most promising sustainable strategies. However, the success of dual relay catalysis could largely be determined by the catalysts' compatibility and balanced kinetics. Previously, we have demonstrated the compatibility between Rh(II) and Pd(0) catalysts.¹ More recently, we also reported an asymmetric dual Rh(II)/Pd(0) relay catalysis, i.e., Rh(II)-catalyzed enantioselective C(sp³)-H insertion/Pd(0)-catalyzed diastereoselective allylation of diazomides.² Herein, we present a Rh(II)/Pd(0) dual relay catalysis for one-pot synthesis of 3,3-disubstituted benzofuran-2-one and indolin-2-one moieties through sequential C(sp²)-H insertion/allylic alkylation of aryl α -diazo compounds.



Poster Presentation : **ORGN.P-185**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Regioselective 2-Sulfonylation of Indole using thiosulfonates

Hyowon Park, Hye-Young Jang^{1,*}

Department of energy systems research, Ajou University, Korea

¹Department of Chemistry, Ajou University, Korea

Indole and its derivatives are known as important intermediates in agrochemical industry and pharmaceutical industry. In particular, 2-sulfonylated indole structure can be found in drugs like SR 33805 oxalate which act as antagonist. But indole's C2 functionalization is known more difficult than C3 functionalization. Therefore, many researchers studied the regioselective synthesis of 2-sulfonylated indole using indole and sulfinate salts. Sulfinate salts have problems like instability and the limited number of commercially available compounds. Compared to sulfinate salts, thiosulfonates are more stable and easily accessible by copper-catalyzed coupling of thiols. In this study, we studied synthesis of 2-sulfonylated indole from indole and thiosulfonates under oxidation conditions. We will discuss detailed optimizations, substrate scopes and the mechanism.

Poster Presentation : **ORGN.P-186**

Organic Chemistry

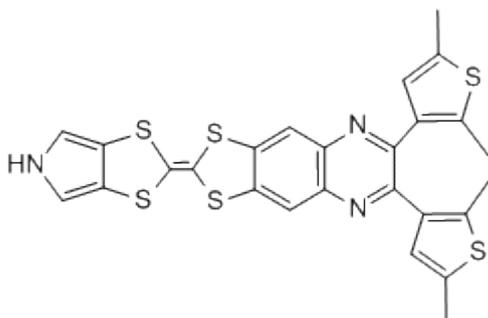
Grand Ballroom, THU 11:00~12:30

Step-wise Protonation Induces Electrochemical Amphotericity and NIR absorption in Quinoxaline-tetrathiafulvalene-pyrroles

Trang Thu Tran, Jung Su Park*

Department of Chemistry, Sookmyung Women's University, Korea

Conjugated donor-acceptor (D-A) systems have been attracted due to their diverse applications such as low-banding gap materials. Among a variety of the electron donating moieties, electron rich tetrathiafulvalene (TTF) moiety is well-known key role for D-A systems. Especially, pyrrole-fused TTF derivatives are used as important building blocks because they can be readily converted to a variety of supramolecular functional materials. On the other hand, quinoxaline, a nitrogen containing bicyclic compound, is widely employed as a versatile electron-deficient building block in various functional electronic materials Here we first present the synthesis of a series of quinoxaline-fused TTF pyrrole derivatives. These derivatives exhibit intramolecular electron transfer (IET) from the TTF pyrrole donor to the protonated quinoxaline acceptor. Upon the protonation, amphoteric redox character, significantly red-shifted ICT band and charge-separated diradical process were observed. These derivatives have been fully characterized by NMR, High Resolution-Mass spectra, and X-ray crystallography. Their electrochemical and photophysical properties are examined by UV-Vis, Fluorescence spectroscopy, CV, DPV and EPR spectroscopy.



Poster Presentation : **ORGN.P-187**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Bioactive Evaluation of Anticancer drug of Breast by Niche chemistry

Songmi Bae, Ju Hyun Song*, Dai Il Jung, Jungtai Hahn¹

Department of Chemistry, Dong-A University, Korea

¹Department of Beauty Care, UI University, Korea

Salicylic acid has been used as an analgesic in the past, but has the disadvantage of disgusting taste. Bayer scientists have synthesized aspirin without side effects through esterification. Our lab got the idea from here. We have developed a way to make drugs with low side effects through the esterification of low molecular weight, and we named it "Niche chemistry". Breast cancer is cancer that develops in breast cells. Typically, the cancer forms in either the lobules or the ducts of the breast. Cancer can also occur in the fatty tissue or the fibrous connective tissue within female breast. To develop new medicine of breast cancer we tried novel synthesis of esters and acid anhydrides by Niche chemistry. Resveratrol as target molecule is a phytoalexin, a class of compounds produced by many plants when they are infected by pathogens or physically harmed by cutting, crushing, or ultraviolet radiation. We report biological activity(MTT assay) of synthesized esters and acid anhydrides.

Poster Presentation : **ORGN.P-188**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

In-vitro and In-vivo Imaging by pH Change depending on Osteoclast Cell Activity

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In-vivo imaging utilizing the near-infrared fluorophores has been widely used to visualize cell and animal metabolic functions. However, visible region fluorescent molecule probes (400-600 nm), commonly used for cell imaging, cannot be simply applied to animal in-vivo imaging because of the challenge of target tissue penetration, as well as their undesirable physicochemical properties for in-vivo imaging. Here, we designed and synthesized a function NIR-pH, which was used as an active osteoclast detection probe to determine as an acid dissociation constants (pKa) of 6 by fluorometry in various pH solutions, with a bone active-targeting moiety, highly photostability, and a fluorescence "OFF/ON" switch and then imaged target osteoclast cell activity by injecting the NIR-pH.

Poster Presentation : **ORGN.P-189**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of ^{64}Cu -labeled Mesoporous Nanoparticles for Comparison of Pretargeting and Non-pretargeting PET Imaging via Bioorthogonal Click Chemistry

Haebin Kim, Kyo-Chul Lee¹, Yong Jin Lee¹, Dong Wook Kim*

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¹Korea Institute of Radiological & Medical Science, Korea

The enhanced permeability and retention (EPR) effect is distinct phenomenon of solid tumors from normal tissues, associated with large gaps between endothelial cells in tumor blood vessels by angiogenesis. Nanoparticles with an appropriate size can be accumulated in tumor cells and target lesions by EPR effects. In this presentation, Mesoporous nanoparticles (MSNs) with 70-90 nm were synthesized and confirmed the shape, size and dispersity by Transmission electron microscopy (TEM). For PET imaging of tumor cells, MSNs were functionalized with aza-dibenzocyclooctynes (DBCO) and labeled with ^{64}Cu ($t_{1/2} = 12.7$ h), the long half-life positron-emitting radioisotopes via bioorthogonal strain-promoted alkyne azide cycloaddition (SPAAC), which is referred as copper-free click chemistry. First, ^{64}Cu was labeled in NODA-GA-PEG₃-N₃ and then ^{64}Cu -NODA-GA-PEG₃-N₃ was employed for confirming the SPAAC reaction with DBCO-MSNs. The results of radio-labeling and click reactions were showed by Radio-TLC.

Poster Presentation : **ORGN.P-190**

Organic Chemistry

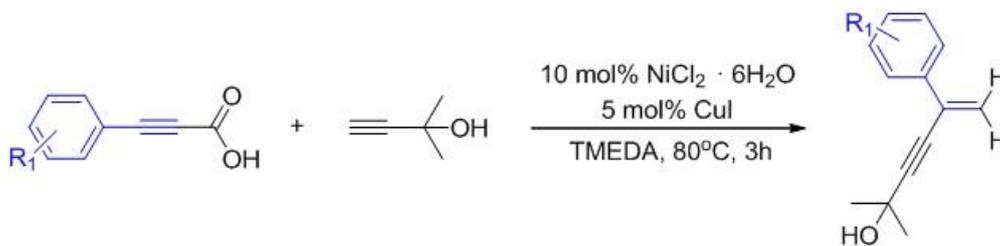
Grand Ballroom, THU 11:00~12:30

Copper-catalyzed decarboxylative coupling reaction of propiolic acid and propargyl alcohol : Unexpected pathway

SeHyeon Han

Chemistry, Chonnam National University, Korea

The development of simple and convenient method for the preparation of aryl alkynoic acids made it easy accessible tool for the introduction of alkynyl group in organic synthesis.¹ In this presentation, we would like to discuss some of our recent research progress towards the decarboxylative coupling reactions of alkynoic acids. Generally, Hay reaction using Ni, Cu, ligand in terminal alkyne is known as diene synthesis method.² However, our experiments using alkynoic acids was to find products in the form of enynes. Enyne were selectively obtained from the reaction with propargyl alcohol and arylpropionic acid in the presence of copper catalyst, nickel catalyst and TMEDA.



- Provide a new method
- One-pot synthesis
- Broad scope of substrate

Poster Presentation : **ORGN.P-191**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Curcumin Derivatives for β -amyloid Plaque Optical Imaging

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The extracellular deposition of β -amyloid ($A\beta$) is considered to be a major pathological property of Alzheimer's disease(AD) brain and the most significant target for molecular imaging. A visualization of cerebral β -amyloid plaques is the most feasible way to diagnose AD. Recently, it has been suggested that the Alzheimer's peptide, $A\beta$, accumulates in the eye. In particular, the rigid conjugated planarity compounds fit into hydrophobic binding channels of $A\beta$ plaques easily. In this study, PEGylated curcumin derivatives were synthesized for binding to $A\beta$ plaques with high photoluminescence and blood circulation. Our synthesized PEGylated curcumin derivatives exhibit near IR fluorescences which are appropriate biological $A\beta$ probes of optical imaging for AD diagnosis.

Poster Presentation : **ORGN.P-192**

Organic Chemistry

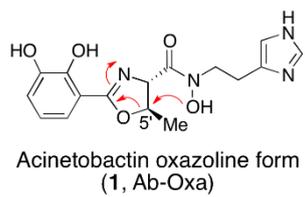
Grand Ballroom, THU 11:00~12:30

Total synthesis and characterization of anguibactin to reveal its competence to function as a siderophore for a gram-negative pathogen, *Acinetobacter baumannii*.

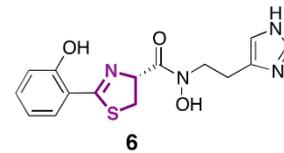
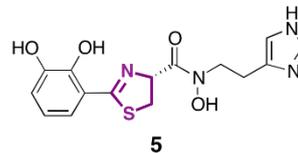
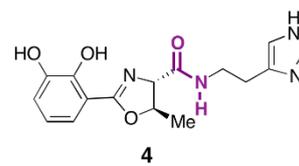
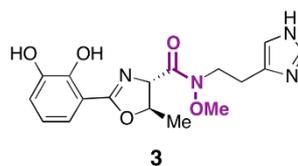
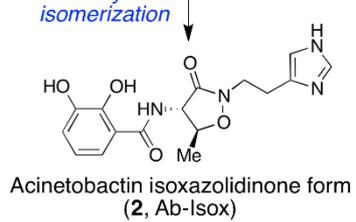
Haeun Lee, Hak Joong Kim*

Department of Chemistry, Korea University, Korea

A gram-negative pathogen, *Acinetobacter baumannii*, has recently emerged as one of the most threatening pathogens, particularly, in the nosocomial settings due to its rapid acquisition of the multidrug resistance. One of the promising strategies to treat this *A. baumannii* infection is the “Trojan Horse” approach in which a siderophore is used as an antibiotic delivery vehicle. Siderophore is a natural product that forms a complex with Fe(III) by which the corresponding bacterium can assimilate this essential mineral from the environment. Acinetobactin is the major siderophore of *A. baumannii*, structurally featuring three potential Fe(III) binding moieties; catechol, hydroxamate, and imidazole groups. Originally, the structure of acinetobactin was reported to possess an oxazoline ring at its core (1), but later this form was found to readily isomerize into its isoxazolidinone derivative (2). Our previous study revealed that indeed the former form is likely to be a more physiologically relevant isoform, and thus more suitable to utilize as an *A. baumannii* targeting antibiotic delivery vector. But, its thermal instability issue should be overcome to progress into further development. In this regard, we have searched for analogues not only thermally stable, but also well mimicking the biological function of acinetobactin oxazoline form (1). This effort led us to synthesize and characterize four analogues (3 ~ 6), and pleasingly anguibactin (5), a siderophore isolated from *Vibrio anguillarum*, was found to fit our need. This presentation details total synthesis and characterization of anguibactin, a suitable surrogate of acinetobactin.



*non-enzymatic
isomerization*



Thermally stable acinetobactin analogues

Poster Presentation : **ORGN.P-193**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Chemical Functionalization on Solid Surfaces with Non-Biofouling Agarose Films for Biomedical applications

Jae Chang Kim, JungKyu Lee*

Department of Chemistry, Kyungpook National University, Korea

Biofouling is the uncontrolled, nonspecific accumulation of biological entities, such as proteins, cells, and microorganisms, on solid surfaces, and adversely affects biological research and applications. This universal and problematic phenomenon results in low signal-to-noise ratios for immunoassays and harmful side effect for biological implants. Thus, it is necessary to introduce functionalities on solid surfaces (e.g., Si/SiO₂, gold, and polymer surfaces), which minimize the unwanted, non-specific adsorption of bioentities as well as improve the device function. Therefore, many studies have been reported how to reduce the nonspecific adsorption of bioentities on the surfaces. Recently, it has been found that non-biofouling coating on biocompatible polymers, such as poly(ethylene glycol) (PEG) derivatives, polysaccharides, and zwitterionic polymers, is one of the best methods to minimize the biofouling on solid surfaces. Herein, we present non-biofouling polymer coatings on gold, silicone oxide, slide glass, graphene, and organic plastic surfaces, using both grafting-from strategy (i.e., surface-initiated, controlled radical polymerization) and grafting-to method (e.g., drop-casting). The formed polymeric coated substrates are characterized by water contact angle, ellipsometric thickness, atomic force microscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy (XPS). Moreover, the non-biofouling performance of the substrates is investigated fluorescence analysis. We believe that the strategy used herein will not only widen the application of non-biofouling coating on solid surfaces to biosensors and medical devices, but also be applicable to various other substrates which need to be functionalized spatioselectively for their applications.

Poster Presentation : **ORGN.P-194**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Characterization of Ultraviolet-Ray Curing type acrylic binder

Eun Ji Park

Advanced material research division, Korea Institute of Footwear & Leather Technology, Korea

Ultraviolet ray curing refers to a process in which a strong ultraviolet energy coming from an ultraviolet lamp gives energy to initiate a chemical reaction with a photoinitiator in a resin to instantaneously turn the monomer or oligomer into a polymer. The ultraviolet curing printing composition is eco-friendly since it does not use any organic solvent in the binder resin synthesizing process and coating process. In addition, short curing times enable mass production and automated processes. Compared with thermosetting resins that require long-time heating at high temperatures, UV curing resins can be cured at room temperature for a short time. So, UV-curable resins can be energy-saving, have high productivity. Also UV-curable resins are environmentally friendly because they are non-solvent type. In this study, ultraviolet curing acrylic binders were prepared and characterized by adhesive strength and creep. Acknowledgement This work was supported by the Technology Innovation Program (or Industrial Strategic Technology Development Program(20000372) funded By the Ministry of Trade, Industry & Energy(MOTIE, Korea)

Poster Presentation : **ORGN.P-195**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Development of a real-time FRET detection system for amyloid- β plaque formation towards therapeutic treatment of alzheimer disease.

Yeon Gyo Hwang, Sang Jeon Chung^{1,*}

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¹*College of Pharmacy, SungKyunKwan University, Korea*

Alzheimer disease (AD) occurs by aggregation of amyloid- β and its accumulation of amyloid- β plaque in the brain can be fatal. Amyloid- β is formed by the cleavage of the amyloid protein precursor (APP). Aggregation of amyloid- β is highly influenced by high concentrations of metal (II) ions in the brain. These metal ions coordinate especially with histidine, glutamic acid, and aspartic acid residues of amyloid- β . There are several methods to detect amyloid- β aggregation, for example, the use of nuclear magnetic resonance (NMR) and transmission electron microscopy (TEM). However, these techniques can be laborious, expensive, and often requires dedicated instruments. To overcome the drawbacks of the aforementioned methods, we designed a fast and reliable system to detect amyloid- β aggregation based on Förster resonance energy transfer (FRET). Real-time imaging of amyloid- β aggregation was achieved using an amyloid- β fragment equipped with an C-terminus unnatural fluorescent amino acid and N-terminus unnatural amino acid. In our design, a C-terminal 1-naphthylamine residue of the amyloid- β fragment act as the FRET donor to the dabcyI residue. However, only upon aggregation of the construct, the FRET pair is in close proximity to allow energy transfer. Consequently, excitation at 330 nm (i.e., 1-naphthylamine excitation maximum) results in quenched significant emission at 430 nm (i.e, 1-naphthylamine emission maximum) by dabcyI absorption upon addition of a metal ion to the artificial amyloid- β fragment. Our FRET based approach allows monitoring of the metal ion induced amyloid- β plaque formation. The developed method may be applicable in the high throughput screening of potential inhibitors of amyloid- β aggregation for the therapeutic treatment of AD.

Poster Presentation : **ORGN.P-196**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Copper-catalyzed synthesis of diaryl disulfides from aryl halides and thioglycolic acid

Kyungmi Kim, Junghyun Chae*

Department of Chemistry, Sungshin University, Korea

C-S bond formation is an important organic reaction in various areas of chemistry, and aryl thiols are usual starting materials in the C_{aryl}-S_{aryl} bond formation. Aryl thiols have high reactivity and are also easily oxidized to diaryl disulfide. Thus, diaryl disulfides are often considered as precursors of the corresponding aryl thiols, which can release aryl thiols in-situ upon reduction. Several studies on the synthesis of diaryl disulfides have been reported, where sulfur powder and metal sulfide such as Na₂S are employed as sulfur sources.¹ In our study, we found that thioglycolic acid, which has many advantages in handling, is an efficient sulfur source for the synthesis of diaryl disulfides under copper catalytic conditions. A variety of diaryl disulfides were prepared in good to excellent yields from substituted aryl iodides and thioglycolic acid by our optimized protocol. Furthermore, the synthesized symmetric diaryl disulfides were demonstrated as the equivalent of aryl thiols in the reaction with aryl halides to produce **asymmetric sulfides**.

Poster Presentation : **ORGN.P-197**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Visible-light Photoredox catalyzed Amides formation from Oxaziridines

GwangSeok Jang, Jin Park¹, Sang Kook Woo^{1,*}

Chemistry, University of Ulsan, Korea

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

Peptide bond is one of most important structure in organic chemistry because of their presence in molecules with drugs, biopolymers, and materials. The traditional approach to amide formation is the condensation of an amine with a carboxylic acid derivative such as acyl halide, anhydride, and by using coupling agents which are generally toxic and/or expensive and generate waste. These methods are associated with significant drawback such as harsh reaction conditions, the use of hazardous reagents, and large amounts of byproducts leading to poor overall atom-economy and difficult purification procedures. We have developed a highly efficient synthetic methods of amide formations from oxaziridines rearrangement by visible light photoredox catalysis.



Poster Presentation : **ORGN.P-198**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Degradable Block Co-polymer with Triarylphosphine as a Junction for Staudinger Ligation

Suhong Park, Yerin Kim, Sol An, Myungwoong Kim*, Dong Wook Kim*

Department of Chemistry, Inha University, Korea

The Staudinger ligation employing azide and phosphine rapidly produce a stable amide bond in the presence of water rather than the products of aza-ylide hydrolysis and has high chemoselectivity, so it has been used extensively in chemical biology for applications including cell labeling, protein immobilization. Through Staudinger ligation, block copolymers possessing triarylphosphine as a junction point enable to decompose or modify one part of block copolymers. Herein we have synthesized degradable block copolymers using poly styrene, methoxy poly ethylene glycol(mPEG), and triarylphosphine. The block copolymers were characterized by ¹H NMR and gel permeation chromatography(GPC). The mPEG part in resultant block copolymers was removed by organic azide compounds through Staudinger ligation. The synthesized block copolymer is anticipated introducing other functionalized molecules.

Poster Presentation : **ORGN.P-199**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Studies on the Synthesis of diarylsulfone using DABSO and Diazonium Salt

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Department of Energy Science and Technology, Myungji University, Korea

¹Department of Chemistry, Myongji University, Korea

The synthesis of diarylsulfone was attempted using diazonium salt as the aryl source and DABSO as a sulfur dioxide (SO₂) surrogate. Various photocatalysts and oxidants were screened, and the reactions were carried out under mild reaction conditions. However, only trace amount of the desired product was obtained, and many side reactions were observed under the reaction conditions. This presentation summarizes our attempts to synthesize diarylsulfone including the application of organophotocatalyst, silver catalyst, and phase transfer catalyst.

Poster Presentation : **ORGN.P-200**

Organic Chemistry

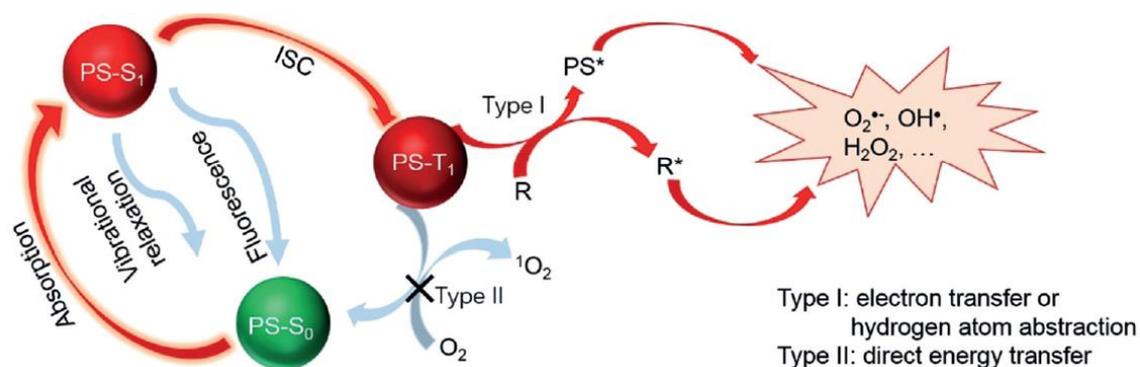
Grand Ballroom, THU 11:00~12:30

Nanostructured Phthalocyanine Assembly for Efficient ROS generation in Photodynamic Therapy

Eunhye Lee, Dayoung Lee, Juyoung Yoon*

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

Recently, Nano-delivery systems in PDT have interesting applications in phototheranostics. But most existing PDT systems utilize PSs that promote ROS generation via type II mechanism, which makes the PDT in oxygen dependent. In studies aimed at developing new strategies for PDT, we made the interesting finding that a novel dot, which is self-assembled from a pure, single Zinc(II) phthalocyanine molecule promotes a highly efficient ROS generation via the type I mechanism. This supramolecular design of NanoPcA displays excellent PDT antibacterial activity. And this can possibly be extended to other molecular assemblies to create PDT systems that possess tunable antibacterial systems activities and to hypoxic tumor PDT. References 1. X. Li, S. Lee, J. Yoon, *Chem. Soc. Rev.* **2018**, *47*, 1174–1188. 2. W. Fan, P. Huang, X. Chen, *Chem. Soc. Rev.* **2016**, *45*, 6488–6519.



Poster Presentation : **ORGN.P-201**

Organic Chemistry

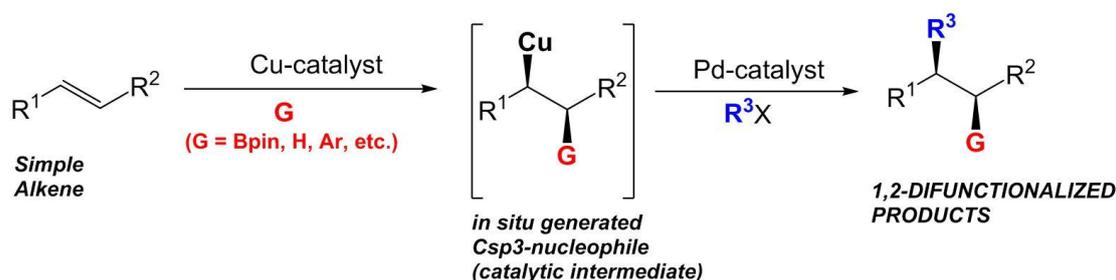
Grand Ballroom, THU 11:00~12:30

Stereoselective Cross-Coupling of Csp³-Nucleophile by Pd/Cu-Synergistic Catalysis

Zakir Ullah, Mu-Hyun Baik*

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Palladium-catalyzed cross-coupling reactions have emerged as an indispensable method for chemical synthesis.¹ The majority of these methods rely on the pregeneration, and often isolation, of the nucleophile component. Synthesis of the requisite nucleophile can often require tedious reaction sequences. Thus, catalytic generation of the nucleophile from simple components and direct cross-coupling would represent an attractive strategy for chemical synthesis.² Herein, we describe a synergistic Pd/Cu catalytic system that allows in situ generation of Cu-based nucleophile from simple alkenes and diboron reagents followed by Pd-catalyzed cross-coupling. As will be outlined below, this strategy offers several advantages over traditional cross-coupling methods. References: 1. Kaitlyn M. Logan, Kevin B. Smith and M. Kevin Brown.; *Angew. Chem. Int. Ed.* 2015, 54, 5228-5231. 2. Kaitlyn M. Logan and M. Kevin Brown.; *Angew. Chem. Int. Ed.* 2017, 56, 851-855.



Poster Presentation : **ORGN.P-202**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

C-N Bond Formation Through Cu-catalyzed Amination of Hetero(aryl)amines to Alkenes

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¹*Department of Chemistry, Kwangwoon University, Korea*

Nitrogen containing compounds are important building blocks because of their interesting and diverse biological activities. One of the most efficient and atom-economy reactions for the synthesis of amines is direct amine addition to multiple C-C bonds using transition metal catalysts. Despite significant advances in this field, the C-N bond formation is still challenging issues for developing more efficient reaction; the use of precious metal catalysts, the use of harsh reaction conditions and controlling selectivities. Therefore, we investigated to develop new and efficient amination reactions of heteroarylamines to alkenes using a copper catalyst. The inexpensive and easy-to-handle Cu salt, readily available phosphine or imidazolium salts, and KOt-Bu were used to generate a Cu amido complex in situ as the catalytic species. Using the catalytic system, we performed regioselective amine addition to -unsaturated ketones and terminal or internal vinylarenes, affording new versatile amine products in good to excellent yields. In addition, we applied our methodology to synthesize a variety of 3-carbonyl-2-substituted quinolin-4(1H)-ones, which are potential intermediates for pharmaceuticals.

Poster Presentation : **ORGN.P-203**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Selective Monitoring and Imaging of Eosinophil Peroxidase Activity with a J-Aggregation Probe

ByungHee Hwang, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

Eosinophils are granulocytic leukocytes that play critical roles in host defense against infections, and are involved in the pathogenesis of asthma and allergic diseases. The cytotoxic activity of granulocytes relies in part on their ability to generate toxic reactive oxygen species (ROS), via haloperoxidases that oxidize halides (X^-) to hypohalous acids (HOX) using hydrogen peroxide. The specific detection of EPO activity requires the difficult distinction between HOBr generated by EPO and HOCl generated by other haloperoxidases. We designed a fluorogenic probe that is halogenated with high kinetic selectivity (>1200:1) for HOBr over HOCl. Heavy atom effects do not quench the dibrominated product because of its self-assembly into emissive J-aggregates that provide a turn-on signal. The probe's response is fast (1 uniquely suited for investigating delicate changes in EPO activity and HOBr levels as pathological biomarkers. We will present applications of this fluorogen to EPO activity assays, dip-stick sensors, fluorescence imaging of EPO activity, assays of oxidative stress in cancer cells, and immune response detection in live mice.

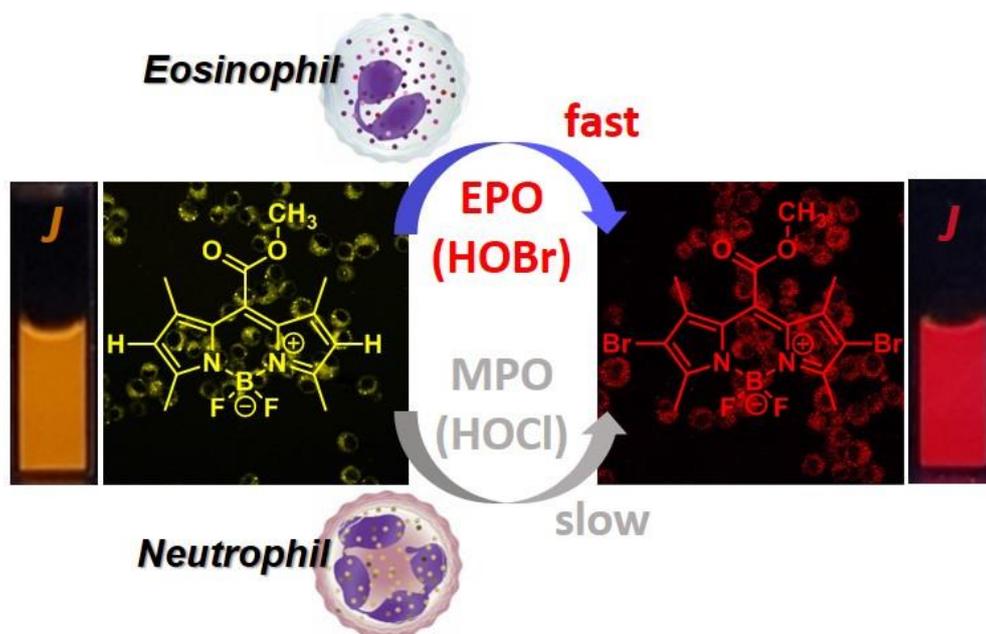


Figure. Proposed sensing mechanism of probe for the monitoring of EPO. The images show confocal fluorescence images of Raw264.7 cells without EPO (left) and with EPO (right) conditions.

Poster Presentation : **ORGN.P-204**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Ratiometric Detection of Cu(II) ion with a Keto-Dipicolylamine Ligand based Fluorescent Probe

Seo Won Cho, Kyo Han Ahn*

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

The environmentally available Cu(II) may go to a higher level due to several human and bacterial activities. The higher levels of environmental Cu(II) cause severe harmful effects not only to the plants, insects, aquatic biota, and microbes but also to human; and ultimately causes an imbalance in the ecosystem and also to the physiological system. Accordingly, detection and quantification of environmental Cu(II) is necessary. Fluorescent detection has its own advantages, and many fluorescent sensing systems are known. As Cu(II) quenches fluorescence, a key challenge in developing fluorescent sensors is to induce fluorescence signal enhancement rather than quenching. A further challenge is to develop probes that provide ratiometric fluorescence changes at two different wavelengths. We have developed such a ratiometric sensing system for Cu(II), which is an acedan-derived dipicolylamine ligand. The probe responded to Cu(II) with a large emission wavelength shift (104 nm) from green to blue in PBS buffer at pH 7.4. The probe was also highly sensitive and thus used to detect trace amounts of Cu(II) ions in nearby river and sea water samples. We performed fluorescence titrations toward Cu(II) and Cu(I) at pH 7.4 and 9.0, respectively, and computational calculations on plausible metal complex intermediates, which provided insights on the sensing mechanism to propose that it involves Cu(II)-promoted enolization and subsequent reduction of Cu(II) to Cu(I). The mechanistic implication guides us to develop other probes and also to reconsider the sensing mechanism involved in the known probes that involving the intramolecular charge transfer upon metal binding.

Poster Presentation : **ORGN.P-205**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A Self-Assembled Fluorophore Aggregate for the Selective Detection of Albumins in Solution and on Electrophoresis Gel

Jiheee Park, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

As one of the most abundant blood plasma proteins, human serum albumin plays a major role in maintaining the oncotic pressures, and transports various ligands. Since the levels of HSA in body fluids are closely associated with various pathophysiological states, the quantitative detection of albumin in biofluids is very important. To date, various methods have been developed for HSA detection. One limitation of organic fluorophores is their general tendency to form aggregates in an aqueous solution, which greatly reduces their fluorescence. This is a drawback to their application in fluorescence-based assays. We exploited this unfavorable property for the highly sensitive and selective detection of serum albumins over other biomolecules. The fluorescent probe 1-SO_3^- initially self-assembles to form nonfluorescent aggregates in aqueous medium, for which the background signal is much lower than that of the monomeric dye (Figure). However, the addition of serum albumin induces the disassembly of the aggregates, and facilitates encapsulation of the probe in the hydrophobic pockets of the protein, which subsequently restricts the rotation of the monomeric dye in the hydrophobic microenvironment. The probe 1-SO_3^- is simple to apply and offers a rapid fluorimetric assay of HSA in either PBS buffer or artificial urine with a high signal-to-noise ratio. Moreover, probe 1-SO_3^- is highly sensitive and selective for detecting native HSA over its denatured forms and other biologically relevant species in aqueous solution. Also, it is a useful tool for the quantitative estimation of HSA in human urine samples and as staining reagent for detecting native HSA on electrophoresis gels.

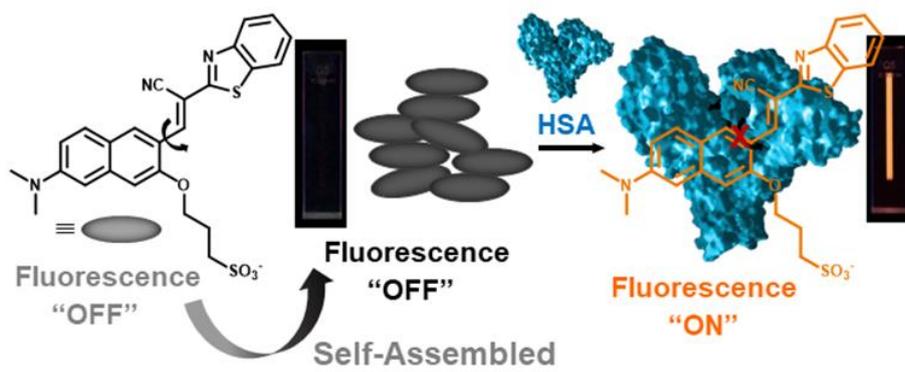


Figure. Structure of probe **1-SO₃⁻**, and the proposed sensing mechanism of **1-SO₃⁻** for HSA.

Poster Presentation : **ORGN.P-206**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Organocatalyzed asymmetric epoxidation of aziridine-2-ylacrylaldehyde : Synthetic application of chiral vicinal epoxyaziridine

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¹Department of Energy Science, Sungkyunkwan University, Korea

(*R*)-phenylethyl aziridine-2-yl-oxirane-2-carbaldehyde bearing both of aziridine and oxirane functional group in a single molecule was prepared from aziridine-2-yl-acrylaldehyde through stereoselective epoxidation with organocatalyst. Chemical and regiospecific ring-opening either at aziridine or at oxirane were successfully achieved. In the presence of NHC catalyst and alcohol, oxirane was converted to alkyl 3-(aziridin-2-yl)-3-hydroxypropionate in high yields which allowed us to determine the stereochemistry of epoxy aziridine. On the basis of this reaction, β -hydroxy- α -amino acid derivative was also achieved in 70% overall yield.

Poster Presentation : **ORGN.P-207**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and analysis of 4,4'-azo-1,2,4-triazole ligand based Metal-Organic Frameworks

Kuktae Kwon, SeungHee Kim, Haneul Park¹, Mingu Han*

Agency for Defense Development, Korea

¹*The 4th R&D Institute 2 directorate, Agency for Defense Development, Korea*

We synthesized energetic metal-organic frameworks (MOFs) by assembly of nitrogen-rich ligand, 4,4'-azo-1,2,4-triazole (atrz) with Cu or Al ions. The crystal structures and thermal behaviors of MOFs prepared were characterized using a single-crystal XRD and DSC, respectively. In addition, their impact and friction sensitivity based on the Bruceton analysis were determined by an OZM BAM fall hammer and friction apparatus.

Poster Presentation : **ORGN.P-208**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

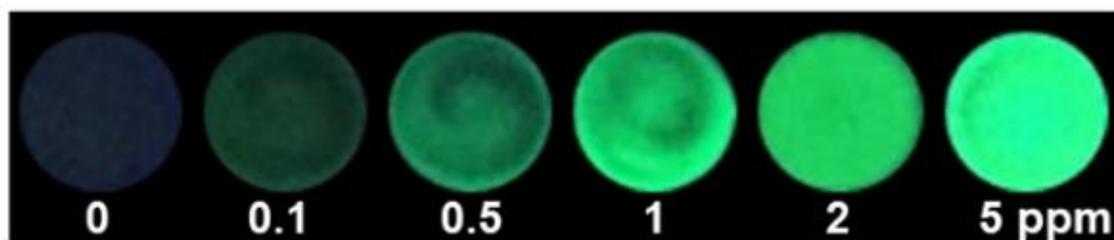
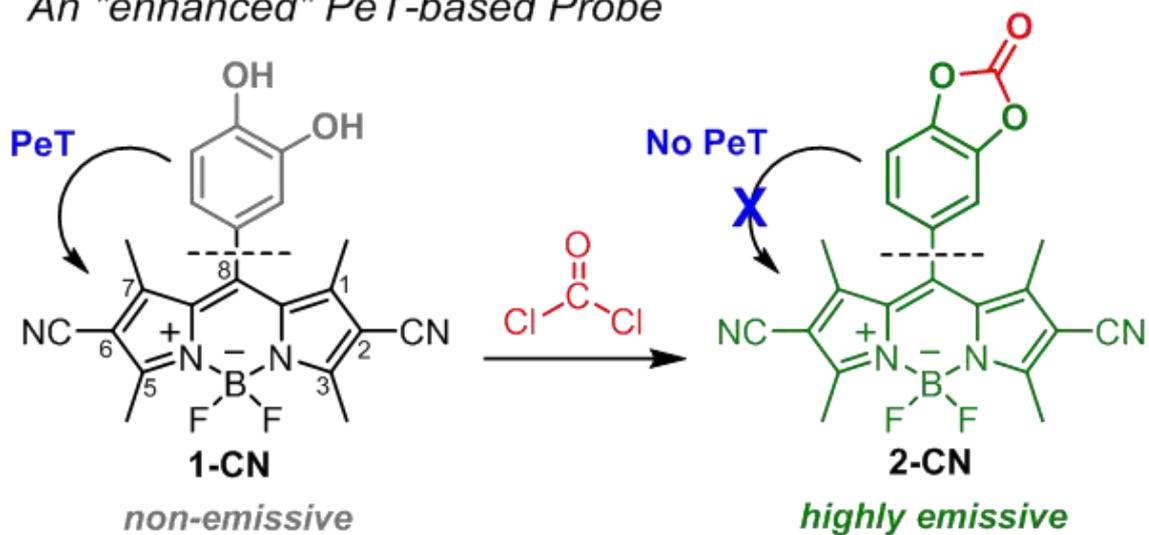
Rapid, Specific and Ultrasensitive Fluorogenic Sensing of Phosgene Based on an Enhanced PeT Mechanism

Dami Kim, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

The dangers of phosgene have spurred the development of methods for its detection and quantification. We will present the rational design and experimental validation of an enhanced PeT-based fluorogenic probe **1-CN** which comprises a BODIPY fluorophore and a catechol quencher at the *meso* position acting as the phosgene reaction site. Strongly electron-withdrawing nitrile substituents at the 2- and 6-positions lower the HOMO energy of the the PeT acceptor (fluorogenic core), at a level such that a rapid PeT quenching occurs from the PeT donor (catechol moiety). However, it is suppressed after the probe **1-CN** is transformed to the cyclic carbonate product **2-CN** by the reaction with phosgene. Due to thermodynamically disfavored PeT process, the product shows bright green fluorescence and can be easily discerned to the naked eye under a hand-held UV lamp (365 nm). **1-CN** responses promptly (within 10 s) and the detection limit was calculated to be as low as 8 pM of triphosgene, corresponding to 2.4 ng/L of phosgene. Furthermore we explored its feasibility under a real threat situation as a portable solid-state platform for the detection of phosgene gas.

An "enhanced" PeT-based Probe



Poster Presentation : **ORGN.P-209**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

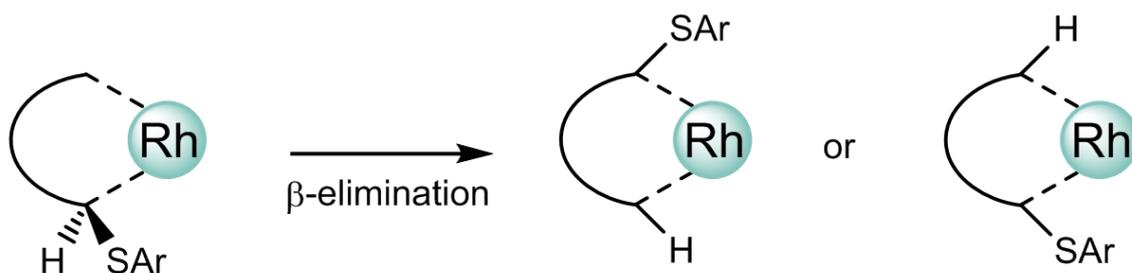
Intramolecular Thioether Migration via the Rhodium-Mediated β -Sulfide Elimination

Dasol Cho, Mu-Hyun Baik^{1,*}

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

The design and implementation of metal-catalyzed higher-order carbocyclization reaction, which combine three or more π -fragments, provides a powerful strategy for target-directed synthesis. In the previous work, we devised a Rh-catalyzed [3+2+1] carbocyclization of carbon- and heteroatom-tethered alkenylenecyclopropanes (ACPs) with CO for the stereo selective construction of cis-fused bicyclohexenones.¹ ACPs, which have an interesting reactivity, undergo two general ring-opening pathways, distal bond and proximal bond breaking.² Computational study demonstrated an unusual reactivity of the distal bond with a low reaction barrier. In this work, we exploit this serendipitous discovery that facilitates an ene-cyclo isomerization of allylic sulfide containing ACPs to five-membered carbo- and heterocyclic rings with concomitant intramolecular thioether migration. The computational and mechanistic studies consistently demonstrate that the inner-sphere transfer of the sulfide, which is remarkable given the propensity for sulfides to poison transition metal catalysts. We envision that this type of rearrangement will prompt the development of related processes given the utility of sulfides in target directed synthesis. Reference 1. Mazumder, S.; Shang, D.; Negru, D. E.; Baik, M.-H.; Evans, P. A. *J. Am. Chem. Soc.* 2012, 134, 20569–20572. 2. Aponte-Guzman, J.; Taylor, E.; France, S. *Org. Lett.* 2014, 16, 3788–3791.



Poster Presentation : **ORGN.P-210**

Organic Chemistry

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Asymmetric Synthesis of cis-5-Aminomethyl-3-(4-methoxyphenyl)- dihydrofuran-2(3H)-one

Sonhwan Kim, Won Koo Lee^{1,*}, Hyun-Joon Ha^{2,*}

chemistry, Hankuk University of Foreign Studies, Korea

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The asymmetric synthesis of (2R,5S)-5-aminomethyl-3-(4-methoxyphenyl)dihydrofuran-2(3H)-one as the most potent selective inactivator of monoamine B was successfully achieved by applying a newly developed synthetic method toward -aminomethyl- -lactone from intramolecular aziridine-ring opening in 63% overall yield from commercial starting material.

Poster Presentation : **ORGN.P-211**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Study on *meso*-ester BODIPY bearing photoactivable *p*-azidobenzyl group

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Chemistry, Kyung Hee University, Korea

¹*Department of Chemistry, Kyung Hee University, Korea*

In our previous work, we reported that the photophysical properties of *meso*-substituted-1,3,5,7-tetramethyl-BODIPY dyes largely rely on the electronic and steric effects of the *meso*-substituents.¹ In particular, the conversion of a *meso*-ester group to the corresponding *meso*-carboxylate of 1,3,5,7-tetramethyl-BODIPY dyes led to the remarkable changes in their spectroscopic properties. By taking advantage of these features, we designed the *meso*-ester-substituted-1,3,5,7 BODIPY (compound **1**) incorporating a light-sensitive *p*-azidobenzyl group. Compound **1** exhibits weak fluorescence emission in diluted solution, but, its absorption and fluorescence emission spectra underwent blue-shifts, along with a significantly enhanced fluorescence intensity upon irradiation with UV-lamp (365nm). Real-time monitoring of the reaction mixture by HPLC-MS and spectroscopic analysis indicated the formation of *meso*-carboxylate BODIPY dye through photoconversion of *p*-azidobenzyl to *p*-aminobenzyl, following by the elimination of *p*-azaquinone methide. We will present the synthesis of compound **1**, its extensive photophysical studies and photoreaction, as well as biological applications.

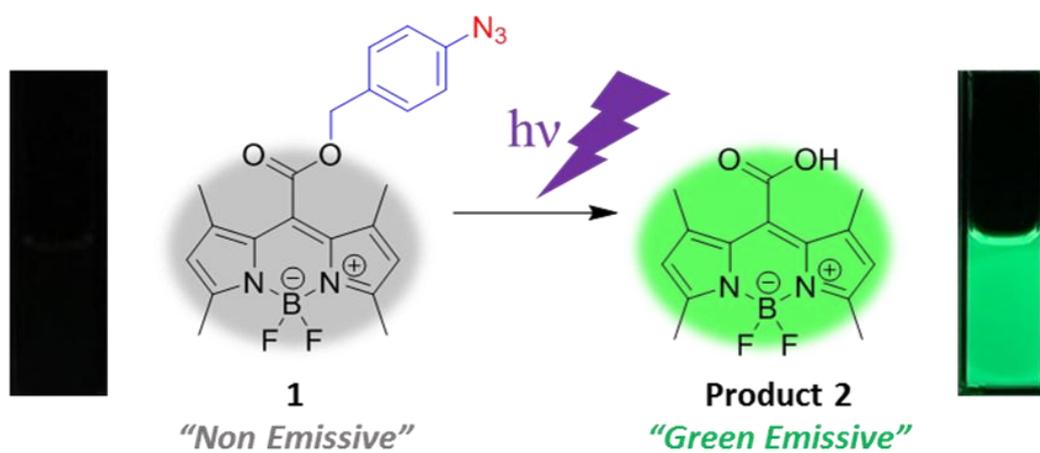


Figure. Scheme of photocleavage of the compound **1** upon UV-irradiation and photographs of **1** before (left) and after (right) UV-irradiation with hand-held UV-lamp (365 nm) for 1 hour.

Poster Presentation : **ORGN.P-212**

Organic Chemistry

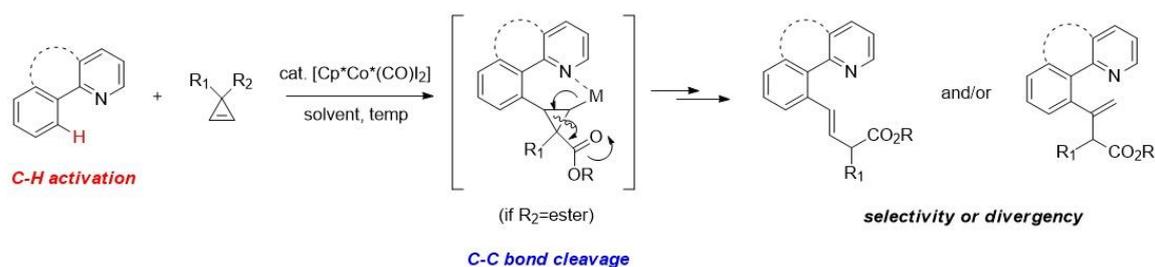
Grand Ballroom, THU 11:00~12:30

Cp*Co(III)-Catalyzed (E)-Selective Alkenylation with Cyclopropenes

Suh Young Choi, Juhyun Kim*

Department of Chemistry, Gyeongsang National University, Korea

From the past decades, transition-metal catalyzed C-H bond activation reaction has undergone groundbreaking development, which makes it possible to achieve various transformations in far more simple way than ever before. However, there are still several limitations to be dealt with. Especially for the C-H alkenylation reactions, two major challenges have still not been resolved; one is that the coupling partners are limited to terminal alkynes and another is controlling E/Z selectivity with broader scope of substrates. In this study, we present cobalt(III)-catalyzed aromatic C-H alkenylation reaction that leads to only E-configured olefins without any double-alkenylation product. The nuclear magnetic resonance (NMR) spectroscopy data of the product indicated the E configuration. By introducing cyclopropane derivatives as olefin moiety, the reaction can be expected to occur via sequential C-H/C-C bond activation, though the reaction mechanism study needs to be further investigated.



Poster Presentation : **ORGN.P-213**

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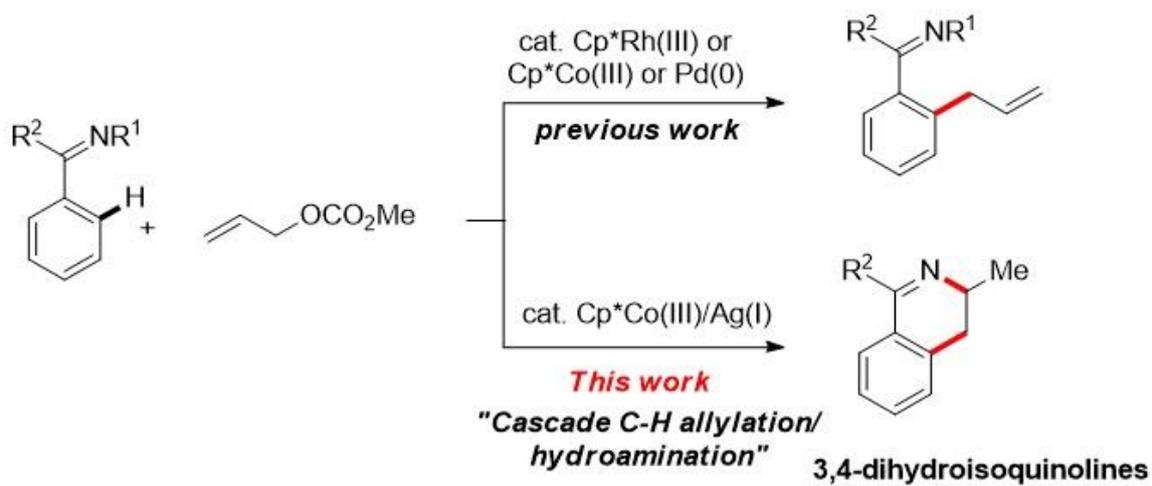
Cooperative Cp*Co(III)/Ag(I)-Catalyzed Cascade C–H Allylation/Hydroamination for the Synthesis of Dihydroisoquinolines

Hyeondae Kim, Juhyun Kim^{1,*}

Department Of Chemistry, Gyeongsang National University, Korea

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

The direct transformation of C–H bonds into useful functional groups offers remarkable atom/step economy of synthetic strategy compared to conventional functional group interconversions. In this context, many effective methods have been developed. Among them, development of a methodology to direct C–H allylation is of great significance and in great demand because the allyl moiety is an exceptionally versatile functional group, offering a wealth of opportunities for further functionalizations. Recently, elegant methods of catalytic C–H bond allylations using first-row transition metal, such as Cp*Co(III) or Mn(I), have been reported. However, Cp*Co(III) catalyzed direct C–H allylation cascading annulation toward the synthesis of valuable N-heterocycles has not been presented. Herein, we report a facile route to access 3,4-dihydroisoquinolines, which are ubiquitous scaffolds that found in many natural products and commercial drugs, via cooperative Cp*Co(III)/Ag(I)-catalyzed C–H allylation and further intramolecular hydroamination, starting from NH imines and allyl methyl carbonates.



Poster Presentation : **ORGN.P-214**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

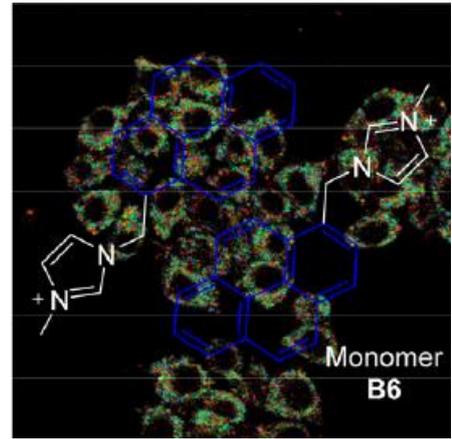
Two-photon fluorescent probes using boranes for specific detecting and imaging Reactive Oxygen Species

Yubin Yim, Sang Jun Park¹, Hwan Myung Kim^{1,*}, Jean Bouffard*, Juyoung Yoon*

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

¹Department of Energy Systems Research, Ajou University, Korea

N-heterocyclic carbene (NHC) borane undergoes oxidative hydrolysis to produce imidazolium salts with outstanding kinetic selectivity for HOCl over other reactive oxygen species (ROS) including peroxides and peroxyxynitrite. Selectivity to HOCl is due to the electrophilic oxidation mechanism of NHC borane as opposed to the nucleophilic oxidation mechanism of arylboronic acid with ROS. Changes in polarity that accompany the conversion of NHC borane to imidazolium salt form the basis of the design of the first fluorescent probe for ROS based on oxidation of B-H bonds by controlling the formation of emissive excimer. Secondly, a ratiometric fluorescent probe, B6S, containing the fluorescent material pyrene and the reactive site imidazoline-2-thione, was also developed for hypochlorite (OCl⁻) detection. Unlike other reactive oxygen species and reactive nitrogen species, B6S is highly specific for OCl⁻. Probes have low detection limits and operate under biological conditions. In addition, the low cytotoxicity of the two probes allows them to effectively utilize OCl⁻ imaging of living cells and tissues using a two-photon microscope. This discovery shows that NHC borane and B6S can serve as probes to explore the biological functions of OCl⁻ in living systems



Poster Presentation : **ORGN.P-215**

Organic Chemistry

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Enhanced Water soluble Dendritic Polymer Photosensitizers for Photodynamic Therapy

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¹*PDT Laboratory, Inje University, Korea*

Photodynamic therapy (PDT) is a treatment that uses a drug, called a photosensitizer (PS) or photosensitizing agent, and a particular type of light. When PSs are exposed to a specific wavelength of light, they produce a form of oxygen that kills nearby cells. It has some advantages as followings: 1) no long-term side effects when used properly, 2) less invasive than surgery, 3) usually takes only a short time and is most often done as an outpatient, 4) high selectivity for targeting in tumor site very precisely, 5) unlike radiation, PDT can be repeated many times at the same site if needed. Recently, our group developed a drug delivery system using gold nanorod (GNR) with anionic PS (sodium salt of purpurin-18) and cationic poly(allylamine hydrochloride) by layer-by-layer method, resulting in formation of GNR-PS complex. This GNR-PS complex is a promising agent for a synergistic (photothermal and photodynamic) therapy (PTT/PDT), in which PTT generates heat as well as operates the PS release which maximize the following PDT activity. The combined dual therapy, PTT followed by PDT, exhibits a significantly higher photocytotoxicity result based on synergistic effect of hyperthermia from PTT as well as singlet oxygen photogeneration from PDT. However, this system needs modification to deliver more amount of PS for enhancement of PDT result. This research presents that synthesis and characterization of new dendritic polymer (2nd generation) type PS contains twelve PSs (methyl pyropheophorbide a) to generate high amount of reactive oxygen species (ROS, such as singlet oxygen) after light irradiation, resulting in enhanced PDT.

Poster Presentation : **ORGN.P-216**

Organic Chemistry

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Asymmetric synthesis of piperidine alkaloids microcosamine A and microgrewiapine A from chiral azirines

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Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

2-Methyl-3-hydroxy-6-alkylated piperidines constitute an important class of natural alkaloids due to their interesting biological and pharmacological properties (anaesthetic, analgesic, antitumor, antibiotic, CNS stimulating biological properties, antihypertensive and antifungal activities etc.). A divergent, new, and highly stereoselective synthesis of 2-methyl-3-hydroxy-6-alkylated piperidine natural products including microgrewiapine A, microcosamine A has been accomplished from aziridine-2(*S*)-carboxylate as chiral pool starting material. Key features of the strategy include the utility of N-methylative aziridine ring opening reaction, intramolecular reductive amination reaction to form the piperidine framework in high yields and Julia–Kocienski olefination to install the triene side-chain.

Poster Presentation : **ORGN.P-217**

Organic Chemistry

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Solvent Free Nucleophilic Fluorination using Ionic Liquid@g-C₃N₄

Parthiban Paramasivam, Dong Wook Kim*

Department of Chemistry, Inha University, Korea

Nucleophilic fluorination is important in the field of radiopharmaceuticals for positron emission tomography (PET) applications. In the continuous search of new catalysts for the betterment in nucleophilic fluorination, here, we introduce an efficient, economic and easily prepared catalyst, IL@g-C₃N₄ (i.e., 1-butyl-3-methylimidazolium ionic liquid at urea derived graphitic carbon nitride) as a potential heterogeneous catalyst with very low concentration of IL. Variety of substrates have been converted into corresponding fluoro analogs using various protocols such as protic, aprotic, aqueous and solvent free conditions as well. This catalyst afford an excellent yield in all conditions in about 1 hour duration with no/negligible or least byproducts. However, an exciting result is, the facile fluorination under solvent free condition at ≤ 100 °C followed by simple separation of the catalyst by flash column. This study highlight that, [Bmim]@g-C₃N₄ as an efficient novel heterogeneous catalyst for nucleophilic fluorination even under green protocol.

Poster Presentation : **ORGN.P-218**

Organic Chemistry

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Morita-Baylis-Hilman reaction of chiral aziridine Aldehyde and distereo selective synthesis of 2,3,4-trisubstituted pyrrolidine

Deepak Singh, Hyun-Joon Ha^{1,*}

Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

The distereo selective MBH reaction of (*R*)-1-((*R*)-1-phenylethyl)aziridine-2-carbaldehyde with acryl acrylate was achieved in stereo selective manner under various reaction onditions by changing the solvent, bases and alcohol additives. The regio specific aziridin ring opening of MBH product by acetic acid yielded 2,3,4-trisubstituted pyrrolidine via aza Michael reaction, which may have utility for the synthesis of various biologically active compounds including Kainic acid.

Poster Presentation : **ORGN.P-219**

Organic Chemistry

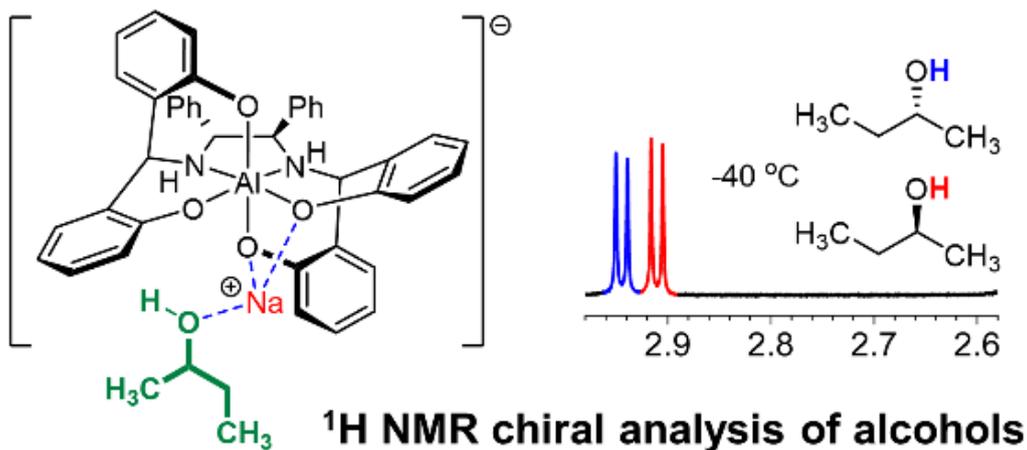
Grand Ballroom, THU 11:00~12:30

Chiral Aluminum Solvating Agent (CASA) for ^1H NMR Chiral Analysis of Alcohols at Low Temperature

Sumin Jang, Kim Hyunwoo*

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

Chiral aluminum solvating agent (CASA) was demonstrated to be a general and efficient reagent for ^1H NMR chiral analysis of alcohols. Sodium salt of CASA (CASA-Na) showed a complete baseline peak separation for various chiral alcohols including primary, secondary, and tertiary alcohols with alkyl and aryl substituents in CD_3CN . Due to the weak intermolecular interaction, ^1H NMR measurement at low ($-40\text{ }^\circ\text{C}$) to ambient temperature was required.



Poster Presentation : **ORGN.P-220**

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A two-photon fluorescence probe for the selective detection of mercury

Gain Baek, Sang Jun Park¹, Hwan Myung Kim^{1,*}, Juyoung Yoon*

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

¹Department of Energy Systems Research, Ajou University, Korea

Abstract Due to the highly toxic property of mercury, the development of novel strategies for the selective detection of mercury in the living cells and tissues is required. In this study, we developed a two-photon fluorescent probe for the selective detection of mercury. When mercury is added to the solution of probe, both the colorimetric change from colorless to yellow and the fluorescence response from blue to green (under 365nm hand-held UV lamp) could be observed using “naked-eyes”. This probe could be effectively utilized to detect mercury from the dual-emission channel in both the living cells and living tissues under two-photon microscopy. Reference 1. K. P. Lisha, Anshup and T. Pradeep, *Gold. Bulletin.*, **2009**, 42, 144.2. M.-P. N. Bui, J. Brockgreitens, S. Ahmed and A. Abbas, *Biosens. Bioelectron.*, **2016**, 85, 280.3. X. Zhang, Y. Xiao and X. Qian, *Angew. Chem. Int. Ed.*, **2008**, 47, 8025 -8029;

Poster Presentation : **ORGN.P-221**

Organic Chemistry

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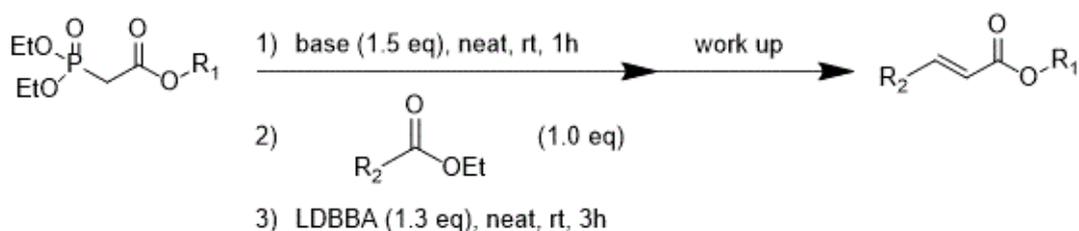
A new method for synthesis of α,β -unsaturated esters using modified Horner–Wadsworth–Emmons (HWE) olefination

Chang whee Hong, Hyun Tae Kim¹, Duk Keun An^{1,*}

chemistry, Kangwon university, Korea

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

For the preparation of α,β -unsaturated esters, Horner–Wadsworth–Emmons (HWE) modification of the Wittig reaction is a widely used method in organic synthesis. Especially, this reaction is popular for stereoselective olefination of carbonyl compounds which are useful in the synthesis of complex natural products. Till date the HWE reaction has been extensively studied¹, However, most of the conditions demonstrated for aldehyde and ketone functional group². To the best of our knowledge, only few reports demonstrated with ester group^{3,4}. Given our interest in finding selective and one pot reactions and the above situation was prompted us to carry out reductive-HWE reaction with ester group. Accordingly, up on treatment of an ester with readily prepared lithium diisobutyl-*t*-butoxy aluminum (LDBBA) and in one pot reaction with phosphate ester, could easily access the desired HWE product under mild conditions (Scheme). 1. *Tetrahedron Letters*, 2018, **59**, 568-5822. *Current Organic Chemistry*, 2015, **19**, 744-7753. *Org. Lett.* 2015, **17**, 5792-5795. 4. *Tetrahedron Letters*. 1986, **27**, 1257-1260



Poster Presentation : **ORGN.P-222**

Organic Chemistry

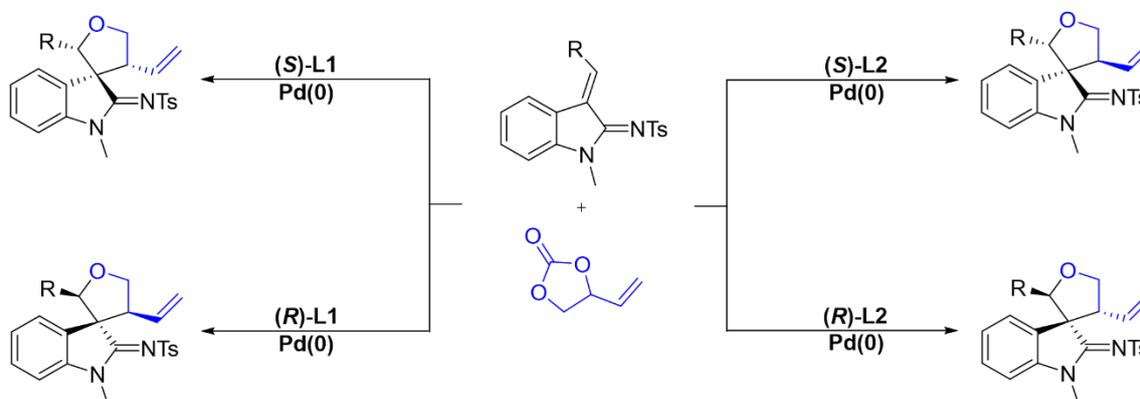
Grand Ballroom, THU 11:00~12:30

Stereoisomeric Spiro-Furanindolines Synthesis via Ligand-Controlled Stereodivergent Palladium catalysis

Hyunji Jeon, Sumin Park, Sang-gi Lee*

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

Stereodivergent (enantiodivergent and diastereodivergent) catalysis is one of the most fascinating yet challenging strategies, because it can allow access to the possible stereoisomers having two or more stereogenic centers. Although the use of different catalysts has been extensively studied for the stereodivergent catalytic reactions, switching solvents or additives often achieved controlling the stereochemical outcomes. Nevertheless, it has not been developed the efficient stereodivergent catalytic reactions, in which both the enantio- and diastereoselectivities can be controlled simply by changing the ligands. In present work, we have investigated the transition-metal-catalyzed ligand-controlled stereodivergent dipolar cycloaddition reactions. The zwitterionic alkoxy π -allyl Pd complex, generated in situ from the vinyl ethylene carbonate, could act as a 1,3-dipole, which may undergo dipolar cycloadditions with stable indolinylidene dipolarophiles. The enantio- and diastereoselectivities of the reactions could be controlled mainly by choice of chiral ligand affording one of the possible stereoisomeric spiro-furanindolines selectively.



Poster Presentation : **ORGN.P-223**

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Stimuli-responsive Self-assembly of Competing Supramolecular Amphiphiles

**Seoyeon Choi, Rahul Dev Mukhopadhyay^{1,*}, Wooseup Hwang², Kangkyun Baek^{3,*},
Kimoon Kim^{2,*}**

Division of Advanced Material Science, Pohang University of Science and Technology, Korea

¹Center for Self-assembly and Complexity (CSC), Institute for Basic Science (IBS), India

²Department of Chemistry, Pohang University of Science and Technology, Korea

³Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Conventional amphiphilic molecules self-assemble due to solvophobic interactions forming well-defined nanostructures, such as rod (1-D) or sheet (2-D) shaped micelles as well as vesicles (0-D) which have potential applications in many fields ranging from materials to medicine. Supramolecular amphiphiles are formed as result of reversible non-covalent interactions and are therefore dynamic in nature. Cucurbit[8]urils are known to form heteroternary supramolecular amphiphiles through charge-transfer or hydrophobic interactions inside their cavity. Depending on the nature of the guest, these supramolecular amphiphiles can be astutely designed to generate redox-responsive (methyl viologen guest) or photoresponsive (azobenzene guest) nanostructures. The competitive exchange between guests, due to different association constant can also be utilized to switch between their 1, 2 and 3-D self-assembled forms. Although there are several examples of stimuli-responsive supramolecular assemblies, only few of them provide a detailed understanding of structural transformations occurring in a complex soup of competing guest molecules. Herein, we demonstrate the formation of these kinds of complex supramolecular nano/microstructures, their stimuli-responsive properties and competitive exchange in solution. The different self-assembled structures formed were investigated using various spectroscopic and microscopic techniques. Efforts to design energy dissipative self-assembling systems from these complex amphiphilic mixtures is in progress. This study may expand the scope of application of supramolecular host-guest chemistry and help us in exploring pathway complexity in self-assembled systems.

Poster Presentation : **ORGN.P-224**

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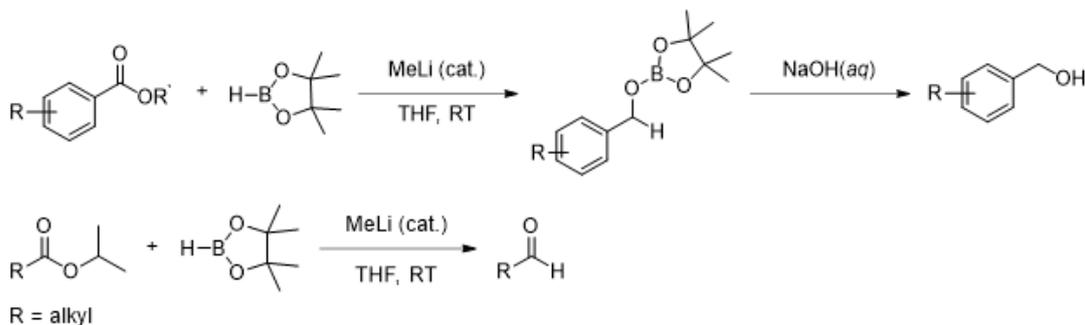
Grand Ballroom, THU 11:00~12:30

Catalyzed partial hydroboration of isopropyl esters to aldehydes.

Su Jin Yang, Jea Ho Kim, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Partial reduction of ester to aldehydes is an economical and important chemical transformation in organic synthesis. DIBALH is a well-known reagent for this transformation under cryogenic conditions (-78 °C). Other than DIBALH, only few methods reported at ambient temperature. On the other hand, number of reports was described for the reduction of ester to alcohol through the metal catalyzed hydrogenation (or) hydrosilylation, (or) with stoichiometric hydride addition (LiAlH_4 or LiBH_4). However, metal catalyzed hydroboration of ester are limited and few examples are reported only with Mg-based catalyst. Given our interest in the partial, selective reductions and the above situation was prompted us to carried out the catalyzed partial hydroboration of esters in one pot. Accordingly, from our recent investigation we could find out the catalyzed partial hydroboration of esters to aldehyde with pinacolborane and alkyl lithium for the first time (Scheme). Further experimental and mechanistic studies are under progress and will be reported in due course.



Poster Presentation : **ORGN.P-225**

Organic Chemistry

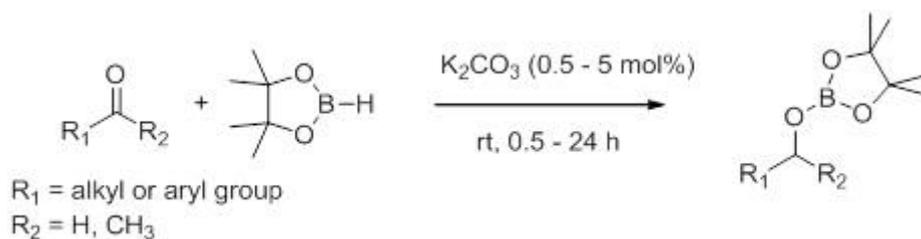
Grand Ballroom, THU 11:00~12:30

Catalytic hydroboration of aldehydes and ketones using K_2CO_3 as a catalyst

Da Hun Ma, Won Kyu Shin, Ashok Kumar Jaladi , Tae Sung Kim, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

In view of economic and environmental concern, the modern synthetic community mainly focusing on the sustainable and green methods as a major targets in recent years. Catalyzed hydroboration of aldehyde and ketones has been identified as significant transformation and well documented with catalyst ranging from transition metals to main group and lanthanide complexes. However, recent reports demonstrate that a catalytic amount of sodium hydroxide, sodium tertiary butoxide, can be used as an efficient initiators of hydroboration. Consequently, considering the importance of hydroboration reactions, we have paid efforts to identify efficient and eco-friendly condition. Here we wish to disclose a facile and economical protocol for the hydroboration of aldehydes and ketones with pinacolborane and bench top K_2CO_3 as catalyst under extremely mild conditions .



Poster Presentation : **ORGN.P-226**

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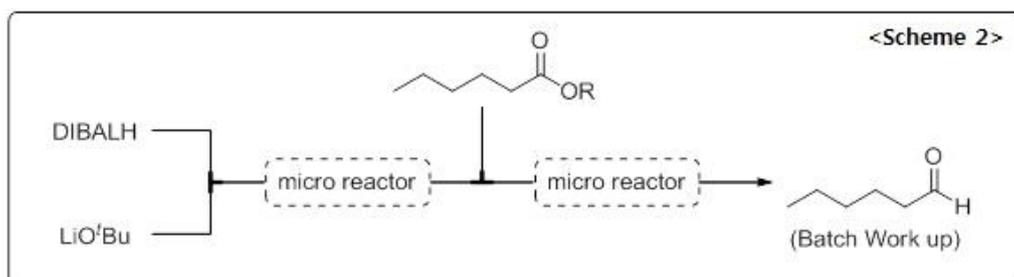
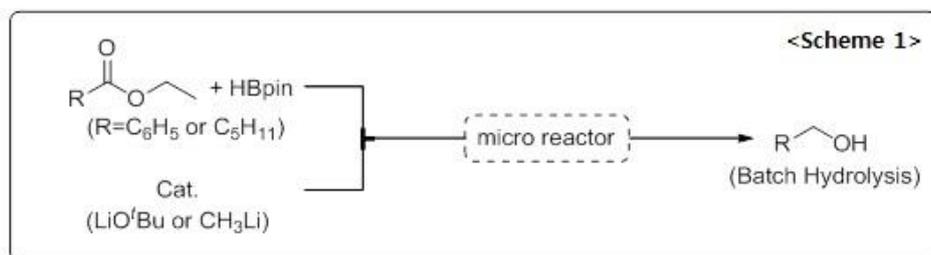
Grand Ballroom, THU 11:00~12:30

Catalytic hydroboration and partial reduction of ester under flow chemistry

Tae Sung Kim, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Due to its high contact efficiency and heat capacity, the flow reactions under micro reactor is known to be highly efficient and reactive than conventional batch systems. Using flow system, with low catalyst load and shorter reaction time an organic reaction can operate with excellent yield. As a result numerous chemical transformations which otherwise difficult to produce in conventional methods was reported by various academies and institutes. As part of our search for efficient reducing agents and selective reductions, and in view of flow technique importance, we made efforts for partial reductions and hydroboration reactions under flow chemistry with ester group. Accordingly an ester group was reduced with LiO*t*-Bu and DIBALH (Scheme 1) and LiO*t*-Bu, MeLi catalyzed hydroboration with pinacolborane (Scheme 2).



Poster Presentation : **ORGN.P-227**

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N-methylative aziridine ring opening and the synthesis of (S)-3-methylamino-3-[(R)-pyrrolidin-3-yl]propanenitrile

Sangyun Na, Won Koo Lee¹, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

¹Department of Chemistry, Sogang University, Korea

The preparation of (S)-3-methylamino-3-[(R)-pyrrolidin-3-yl]propanenitrile (1), a key fragment of fluoroquinolone antibiotic PF-00951966 and others was achieved by N-methylative aziridine ring opening, addition of methyl group at the ring nitrogen, and ring-opening via a cyanide nucleophile in a single operation starting from bicyclic (R)-2-[(R)-pyrrolidine-3-yl]aziridine. The starting compound was elaborated from stereoselective conjugate addition of nitromethane to (R)-aziridine-2-yl acrylate followed by selective reduction without breaking the aziridine ring.

Poster Presentation : **ORGN.P-228**

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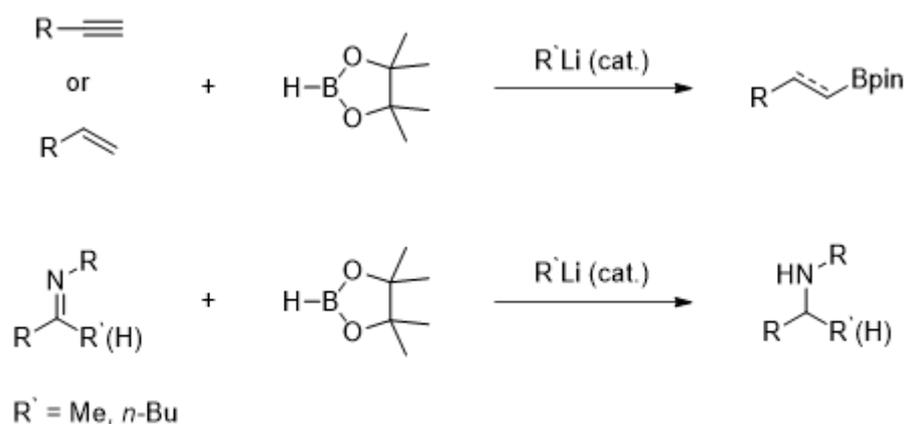
Grand Ballroom, THU 11:00~12:30

Novel catalytic hydroboration of alkene, alkyne and imine with pinacolborane and alkyl lithium as catalyst.

Su Jin Yang, Jea Ho Kim, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

The alkene and alkyl boronates are versatile building blocks in various metal mediated cross-coupling reactions. Hydroboration is an effective method for the preparation of organoboronate compounds. In recent days much attention is focusing on catalyzed hydroborations, leading to its rapid application starting from transition metals to main group-alkaline earth elements, and lanthanide complexes. In addition to alkene hydroboration, the catalytic hydroboration of carbonyl compounds also an important chemical transformation. Practically, identification of effective and eco-friendly condition for catalyzed hydroboration of chemically less reactive substrates (like ester and imine) is challenging. With this aim, we focused on the catalytic hydroborations without the use of toxic and costly metal complexes in a sustainable manner. The present abstract is for alkyl lithium catalyzed hydroboration of alkenes, alkynes and imine with pinacolborane (Scheme).



Poster Presentation : **ORGN.P-229**

Organic Chemistry

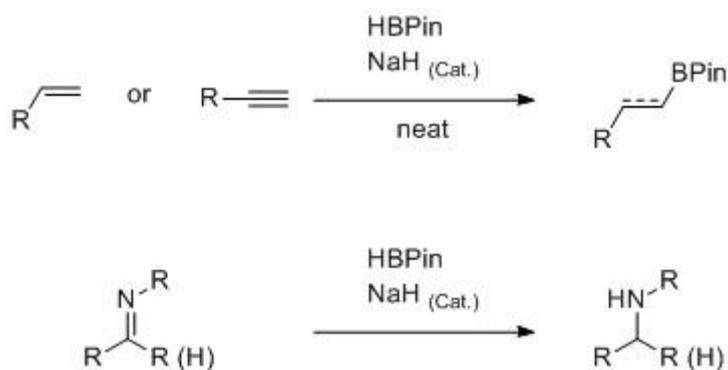
Grand Ballroom, THU 11:00~12:30

Sodium hydride catalyzed hydroboration of unsaturated hydrocarbons and imines

Hanbi Kim, Won Kyu Shin, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Amines have widespread applications as solvents, textile additives, disinfectants, and intermediates for pharmaceuticals. Synthesis of secondary amines through C=N bond reduction is a straight forward and often used in organic synthesis. The traditional hydrogenation with transition metals is well examined. Whereas, hydride reduction with LiAlH₄ or NaBH₄ is unattractive due to their poor yields and product selectivity. Therefore, efficient and sustainable conditions with commercial, inexpensive catalyst are still needed. In addition, the organoboranes obtained from hydroboration are remarkably valuable precursors for various chemical transformations. The catalyzed hydroboration of alkenes and alkynes are economical and efficient reactions than stoichiometric reactions. In this regard, various transition, main group elements have been identified. During the course of our search for efficient and selective reductions, we have identified selective hydroboration of aldehydes and ketones using commercial NaH as catalyst. In continuation, with modified and optimal conditions, we successfully obtained catalyzed hydroboration of alkenes, alkynes, and imines with pinacolborane and NaH under mild reaction conditions.



Poster Presentation : **ORGN.P-230**

Organic Chemistry

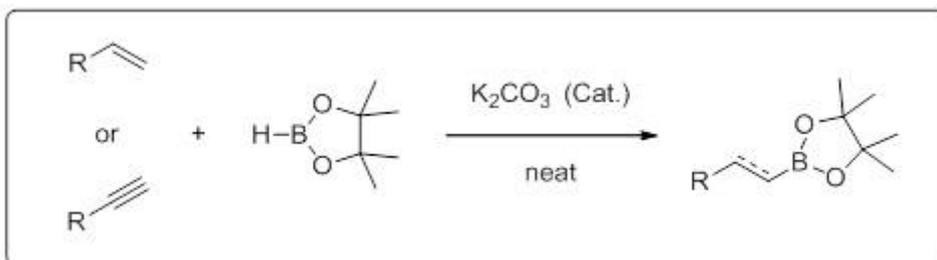
Grand Ballroom, THU 11:00~12:30

Potassium carbonate catalyzed hydroboration of alkenes and alkynes

Tae Sung Kim, Da Hun Ma, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

From the past to the present, hydroboration of unsaturated hydrocarbon compounds using various catalysts has been reported. In recent years, studies have been made to utilize an economical and environmentally catalyst for hydroboration in order to increase the efficiency of the reaction. For the first time In this study, alkenes and alkynes were hydroborated in the presence of pinacolborane under slight heating conditions using potassium carbonate (K_2CO_3) as a catalyst. Potassium carbonate (K_2CO_3) is a cheap and commercially available reagent which is economical.



Poster Presentation : **ORGN.P-231**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Conjugated polymers based on benzimidazole derivatives as electron-deficient units for organic solar cells

Raquel Kristina Leoni Tumiar, Juae Kim, Hongsuk Suh*

Department of Chemistry, Pusan National University, Korea

Polymer solar cells (PSC) have attracted many attentions because of its advantages such as lightweight, inexpensive to fabricate, and good flexibility. We designed new electron donor-acceptor conjugated polymers composed of electron-rich group, thienylthienoindole (TTI) for organic solar cells. Synthesized conjugated polymers, **HS-5618**, **HS-5611** and **HS-5616 H/C** were synthesized by Stille polymerization and the photovoltaic properties of the device were measured. These polymers consist of thienylthienoindole (TTI) as electron rich groups and benzimidazole derivatives as electron deficient groups. The device composed of **HS-5618** showed a V_{OC} of 0.6 V, a J_{SC} of 5.975 mA/cm², and a fill factor (FF) of 31.86%, giving a power conversion efficiency of 1.14%. The device composed of **HS-5611** showed a V_{OC} of 0.7 V, a J_{SC} of 6.983 mA/cm², and a fill factor (FF) of 38.54%, giving a power conversion efficiency of 1.88%. The device composed of **HS-5616 H** showed a V_{OC} of 0.47 V, a J_{SC} of 0.486 mA/cm², and a fill factor (FF) of 28.56%, giving a power conversion efficiency of 0.07%. The device composed of **HS-5616 C** showed a V_{OC} of 0.77 V, a J_{SC} of 2.91 mA/cm², and a fill factor (FF) of 30.90%, giving a power conversion efficiency of 0.69%.

Poster Presentation : **ORGN.P-232**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

(Z)-Selective Formation of Trisubstituted Olefins from the Ruthenium-Catalyzed Dehydrative C–H Coupling of Phenols with Ketones

Manoj Mane, Mu-Hyun Baik^{1,*}

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

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

The carbon-carbon bond forming reactions are an important tool in the field of organic chemistry. In general, traditional Friedel-Crafts alkylation, Wittig type coupling reactions, McMurry and Tebbe-Petasis olefination reactions are extensively used for the construct the C–C bond.¹⁻³ However, these methods have the drawback of requiring the stoichiometric amount of ylide or transition metal reagents results in the formation of a copious amount of toxic and wasteful byproducts. In this regards to overcome this disadvantage, employed the cationic ruthenium hydride catalyst, $[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$. Herein, successfully used the ruthenium-hydride catalyst for the dehydrative C–H coupling of phenols with ketones to form the trisubstituted olefin product. By combined experimental and computational analyses to establish a detailed mechanism as well as to elucidate the origin of stereoselectivity for the olefination reaction. To understand the reaction mechanism and to elucidate the origin of (E)/(Z)-stereoselectivity, we turned to the computational study. The computational study analysis revealed that the stereoselective formation of (Z)-olefins results from an unfavorable steric interaction between the substrate substituents and the axial carbonyl ligand of the Ru-catalyst during the migratory insertion step. The catalytic method features a direct catalytic C–H olefination method of ketones with phenols without employing any reactive reagents or forming any wasteful byproducts. References(1) Fürstner, B. A.; Bogdanovic, B. *Angew. Chem., Int. Ed. Engl.* 1996, 35, 2442–2469. (2) Ephritikhine, M. *Chem. Commun.* 1998, 2549–2554. (3) Hartley, R. C.; Li, J.; Main, C. A.; McKiernan, G. J. *Tetrahedron* 2007, 63, 4825–4864.

Poster Presentation : **ORGN.P-233**

Organic Chemistry

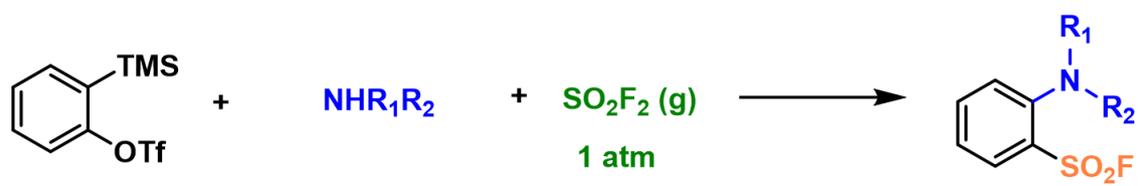
Grand Ballroom, THU 11:00~12:30

Efficient synthesis of substituted *o*-aminoarenesulfonyl fluorides through aryne formation followed by sulfuryl fluoride incorporation

Jungmin Kwon, Byeong Moon Kim*

Division of Chemistry, Seoul National University, Korea

Sulfonyl fluorides have found significant use in chemistry and chemical biology.¹ They have attracted much attention due to their characteristic balance between stability and chemoselectivity.² Despite the importance of sulfonyl fluorides, however, direct synthetic approaches toward benzenesulfonyl fluorides have been still limited. Recently, Willis group demonstrated a palladium-catalyzed one-pot synthesis of sulfonyl fluorides from aryl and heteroaryl bromides.³ This process involves transition-metal catalyzed sulfonylation of aryl and heteroaryl bromides using DABSO as a SO₂ source, followed by one-pot fluorination of the resultant sulfinic acid with an electrophilic fluorine source. The tolerance is noteworthy, nevertheless, an alternative, transition-metal-free synthetic procedure would be more desirable than the two-step reactions involving sulfonylation followed by fluorination. We herein report the development of a new and efficient protocol affording 2-diakly-, 2-alkylaryl- or 2-diarylamine-substituted arenesulfonyl fluorides without using metal-based reagents. This novel transition-metal-free multicomponent coupling reaction involves arynes, secondary amines, and sulfuryl fluoride. Nucleophilic attack of a secondary amine on *in situ* generated aryne followed by reaction with sulfuryl fluoride works efficiently under mild conditions, providing diverse *o*-aminoarenesulfonyl fluoride derivatives in good to excellent yields. We have demonstrated that zwitterionic intermediate formed from the reaction of aryne with secondary amine can capture sulfuryl fluoride as an electrophile, offering a unique and practical protocol for the synthesis of *o*-amino substituted arenesulfonyl fluorides. **Reference** 1. Narayanan, A.; Jones, L. H. *Chem. Sci.* **2015**, *6*, 2650. 2. Dong, J.; Krasnova, L.; Finn, M. G.; Sharpless, K. B. *Angew. Chem., Int. Ed.* **2014**, *53*, 9430. 3. Davies, A. T.; Curto, J. M.; Bagley, S. W.; Willis, M. C. *Chem. Sci.* **2017**, *8*, 1233.



Poster Presentation : **ORGN.P-234**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

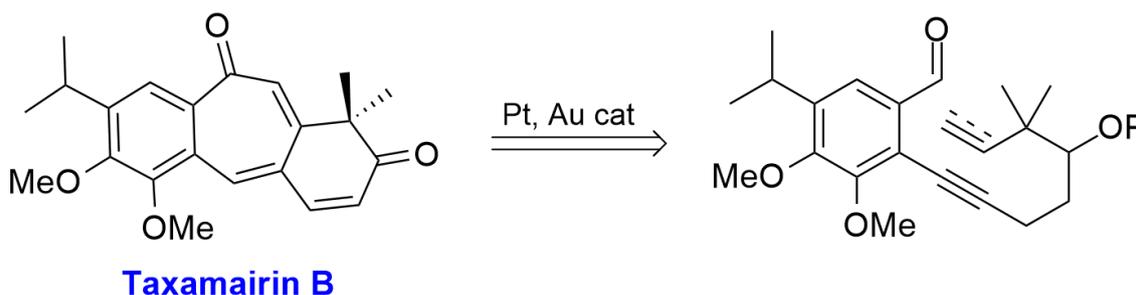
Gold and Platinum Catalyzed Cycloisomerization Strategy for the Synthesis of Icetexane Diterpenoids: Total Synthesis of Taxamairin B

Le Thuy Quynh, Seonmi Lee¹, Juyeon Kang¹, Chang Ho Oh^{1,*}

Chemistry department, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Many structurally novel and biologically active icetexane- diterpenoids isolated from various species in the *Salvia* genus. The subclass of highly unsaturated icetexanes are Taxamairin A and B which were isolated in 1987 from *Taxus mairei*. An initial survey of Taxamairin A and B was identified inhibitory activity against hepatoma (liver tumor) cells^[1]. Here in, we will report general approaches to the tricyclic core of the icetexane natural products via the cycloisomerization of enynal and diynal by utilizing platinum, and gold-catalyst. This strategy provides an efficient synthesis to construct the 6-7-6 tricyclic- key skeletons which could be applied to construction of icetaxanes as representing Taxamairin A and B .



Poster Presentation : **ORGN.P-235**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Lophirone F

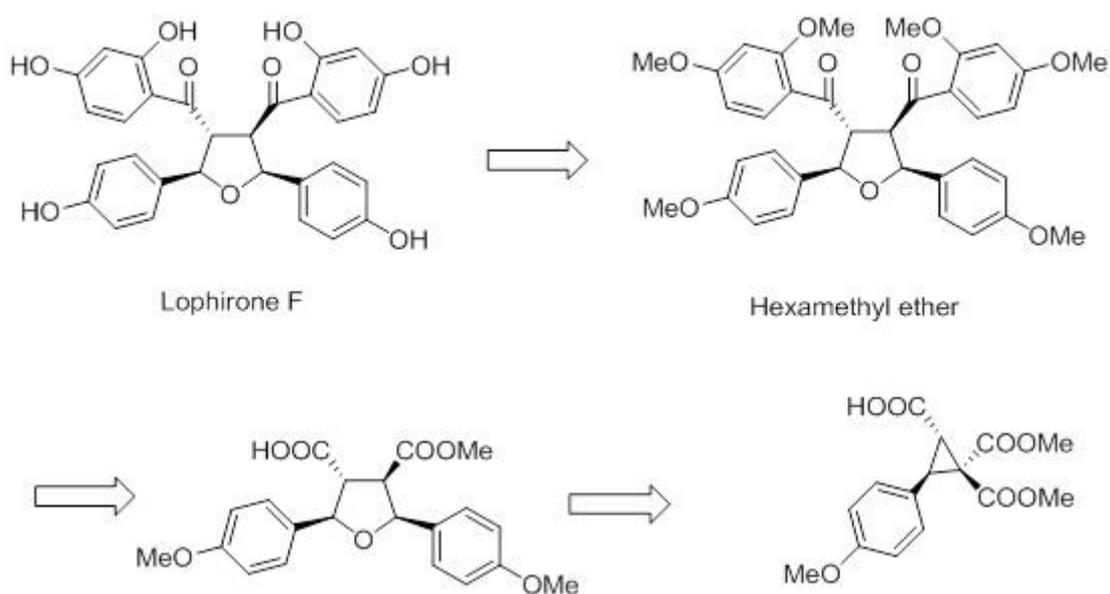
Tien Dung Do, Minh Hoang Le¹, Chang Ho Oh^{2,*}

Chemistry, Hanoi University of Science, Vietnam

¹*Chemistry, Hanyang University, Vietnam*

²*Department of Chemistry, Hanyang University, Korea*

Lophirone F has been isolated from the stem bark of *Lophira lanceolata* growing in the tropical forests of Africa. We have successfully synthesized its hexamethyl ether with reasonable yield by taking advantage of the [3+2] cyclization between a substituted cyclopropane and p-methoxybenzaldehyde. We are now trying to find a mild condition for the demethylation towards Lophirone F, which causes no effect to the THF core. This work also launches an approach towards the syntheses of THF-based natural products that we are currently engaged with.



Poster Presentation : **ORGN.P-236**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Total synthesis of cytotoxic active natural products from *Lindera* aggregate via MBH ester

Dong Guk Nam, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Secobutanolide and Subamolide series has been reported with their excellent biological cytotoxicity. These material has excellent activities on cancer cell lines. And Morita-Baylis-Hillman (MBH) ester carbon frameworks can be precursors for these structures. Our group reported asymmetric synthesis of (z)- β -iodo Morita-Baylis-Hillman ester with oxazaborolidinium catalyst (COBI). With MBH ester precursors, secobutanolide and subamolide series are successfully synthesized in several steps include geometry selective iodo-isomerization. This synthesis was first chiral example of these materials with good yield and excellent enantioselectivity.

Poster Presentation : **ORGN.P-237**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Catalytic Asymmetric Synthesis of Cyclobutanones via Tandem Cyclopropanation/SemiPinacol Rearrangement

Su Yong Shim, Yuna Choi, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Cyclobutane derivatives are found in a wide range of natural products and important building blocks in organic synthesis since they can be converted to various organic compounds through ring opening or ring expansion reactions due to their inherent ring strain. Especially, cyclobutanone is one of the most versatile chemical candidates for the functionalized cyclobutanes through various chemical transformations. In this research, we report enantioselective synthesis of cyclobutanone catalyzed by chiral oxazaborolidinium ion (COBI) from α -silyloxyacroleins and α -alkyl or α -aryl diazoesters via tandem cyclopropanation/semipinacol rearrangement. Various cyclobutanones possessing chiral β -quaternary carbon center were obtained in high yield (up to 91%) with excellent enantio- and diastereoselectivity (up to 98% ee and up to > 20:1 dr). In addition, support for the proposed mechanism of this reaction was provided by isolating the intermediate 1-formyl-1-silyloxycyclopropane and confirming its stereoselective trans-formation to cyclobutanone.

Poster Presentation : **ORGN.P-238**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Disubstituted α -Pyrones and α -Pyridones via Metal-Mediated Cascade Reactions

Juyeol Lee, Hui Jin, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

α -Pyrone and α -Pyridone derivatives exist abundantly in nature, and take part in many biological processes. Therefore, efficient synthesis of substituted α -pyrones and α -pyridones have attracted much attention of many chemists. In this research, 6-ester-substituted α -pyrones and α -pyridones are successfully synthesized through organocatalytic Michael addition-lactonization of β,γ -unsaturated α -keto ester or β,γ -unsaturated α -imino ester with dithiomalonate followed by mercury(II) acetate-induced hydrolysis-decarboxylation-dehydrogenation reaction cascade.

Poster Presentation : **ORGN.P-239**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of a Label-Free Förster Resonance Energy Transfer Probe for the Detection of Mouse double minute 2 homolog (MDM2) and B-cell lymphoma 2 (Bcl-2).

A Ro Han, TaeJin Lee¹, Ju Hwan Kim², Hyo Jin Kang³, Sang Jeon Chung^{4,*}

Department of Pharmacy, Sungkyunkwan University, Korea

¹*Abtis, Korea*

²*R&D Team, AbTis co.Ltd., Korea*

³*Department of Chemistry, Dongguk University, Korea*

⁴*College of Pharmacy, SungKyunKwan University, Korea*

Tumor suppressor is a key factor in cancer cell suppression and is present at a low concentration in normal cells. However, when normal cells receive a cellular stress, such as DNA damage, hypoxia, ribonucleotide depletion or telomere erosion, causes activation of various tumor suppressors. In conclusion, depending on the cellular stress and cell type, the activation of tumor suppressor can lead to various responses. One of the important tumor suppressors, p73(p53 family) acts as a transcription factor, and is able to activate many genes to induce these specific functions and cancer suppression. p73 is an attractive therapeutic target in oncology because its tumor-suppressor activity can be stimulated to eradicate tumor cells. In this experiment, we synthesized probe in which a portion of the p73 peptide sequence was modified to detect MDM2 and Bcl-2. MDM2 and Bcl-2 play a crucial role in the regulation of cancer growth regulation. MDM2 is an important negative regulator of the p73 tumor suppressor. After binding to p73, it inhibits its transcriptional activity, favors its nuclear export and stimulates its degradation. The inhibition of the p73–MDM2 interaction is an attractive strategy to activate p73-mediated apoptosis in tumors with overexpressed MDM2. Another target is Bcl-2 that regulate cell death(apoptosis), by either inducing (pro-apoptotic) or inhibiting (anti-apoptotic) apoptosis. The synthesized probe has a label free Förster Resonance Energy Transfer (FRET) signal because it has a tryptophan and a fluorescent dye. Therefore, the fluorescence signal of FRET is turned off and detection of MDM2 and Bcl-2 became possible. The label free FRET-based probe can be used for cancer diagnosis through easy screening of MDM2 and Bcl-2 oncogenic proteins.

Poster Presentation : **ORGN.P-240**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Asymmetric Allylation Reaction Catalyzed by a Chiral Lewis acid

Taehyeong Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

The asymmetric allylation of aldehydes is one of the carbon–carbon bond-forming reactions in chemical synthesis and has been a testing ground for new asymmetric methodology. Enantiomerically pure homoallylic alcohols are common synthetic intermediates, and are typically generated by allylmetal-aldehyde addition reactions. A novel strategy has been developed for an enantioselective allylation reaction of various aldehydes with aromatic and aliphatic groups catalyzed by a chiral lewis acid. The reaction with allylreagents provides homoallylic alcohols in good yields and with high enantioselectivity. Therefore, this reaction will show promising utility in various other challenging chemical reactions and conspicuous biological activity.

Poster Presentation : **ORGN.P-241**

Organic Chemistry

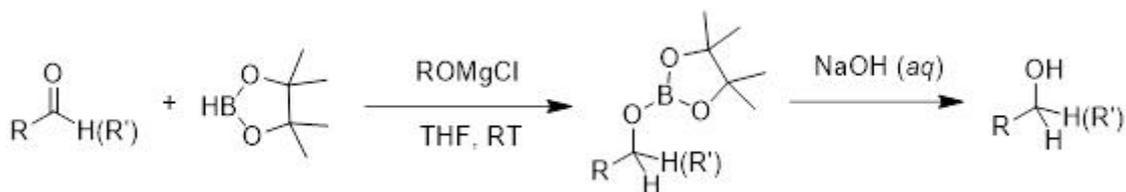
Grand Ballroom, THU 11:00~12:30

New and efficient catalytic hydroboration using pinacolborane and chloroalkoxymagnesium as catalyst.

Jea ho Kim, Ashok Kumar Jaladi , Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

In view of environmental pollution and cost of chemical transformation, catalyzed reactions have gained much beneficial than stoichiometric reductions. Thus, leading to its rapid applications with transition metal complexes and main group elements. Hydrofunctionalization, such as hydroboration is one such transformation due to their mild nature and versatile utility as building blocks for various chemical reactions. In addition, reduction of carbonyl groups like aldehyde and ketone to alcohol is a promising transformation in organic synthesis, with industrial applications. We made efforts for catalyzed hydroboration for carbonyl compounds and succeeded with commercial bench top catalyst with good yields. Here the present abstract demonstrate the catalyzed hydroboration of various carbonyl compounds using magnesium chloride and ethoxide with pinacolborane under mild reaction conditions (**Scheme**).



Poster Presentation : **ORGN.P-242**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Organic solar cells using conjugated polymer based on thiazolo[5,4-b]pyridine as electron-deficient groups

Raquel Kristina Leoni Tumiar, Piao Junying, Juae Kim, Hongsuk Suh*

Department of Chemistry, Pusan National University, Korea

2-{4-[4,6-Bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-b]pyridine (pPTP) as electron-deficient units were synthesized for novel electron donor-acceptor conjugated polymers. Polymers, pPTPTTI, pPTPBDTT-EH, pPTPBDT-EH and pPTPBDT-12, were made up of 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI), or benzo[1,2-b;3,4-b']dithiophene (BDT), or 4,8-bis(5-thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene (BDTT) as electron donor units and pPTP as electron acceptor units was designed. The pPTP as a strong electron-withdrawing units was at the para location of the pyrimidine backbone. The OPV was made up of pPTPTTI and PC₇₁BM (1:1) with 3% CN additive indicated a fill factor (*FF*) of 0.31, a *J*_{SC} of 4.41 mA/cm², a *V*_{OC} of 0.83 V, denoting a power conversion efficiency of 1.13%.

Poster Presentation : **ORGN.P-243**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

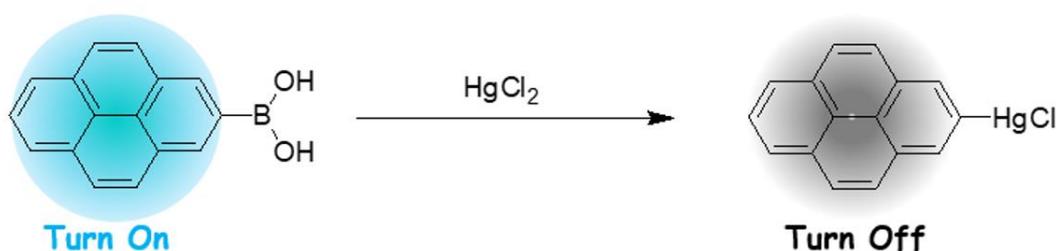
A Simple Boronic Acid-Based Fluorescent Sensor for Sensitive Detection of Hg(II) ion

Sun Woo Lee, Seoung Ho Lee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

Mercury has been widely applied in various fields, such as chemistry, medicine, and biology. Because its wide availability in many areas gives rise to the increase of diseases related to mercury poisoning, it has been considered as one of the most dangerous pollutants in environment. In this work, we have developed a simple boronic acid based fluorescence sensor (Py-mBOH) for selective and sensitive detection of Hg(II) ion where Hg(II) ion ensues a fast transmetallation of Py-mBOH causing drastic reduction of it fluorescence. For the environmental applications, mercury contamination in tap water was successfully monitored in nano-molar concentration levels.



Blacks Li⁺ Na⁺ K⁺ Cs⁺ Mg²⁺ Ca²⁺ Sr²⁺ Ba²⁺ Mn²⁺ Fe²⁺ Fe³⁺ Co²⁺ Ni²⁺ Cu²⁺ Ag⁺ Zn²⁺ Cd²⁺ Hg²⁺ Sn²⁺ Pb²⁺



Poster Presentation : **ORGN.P-244**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

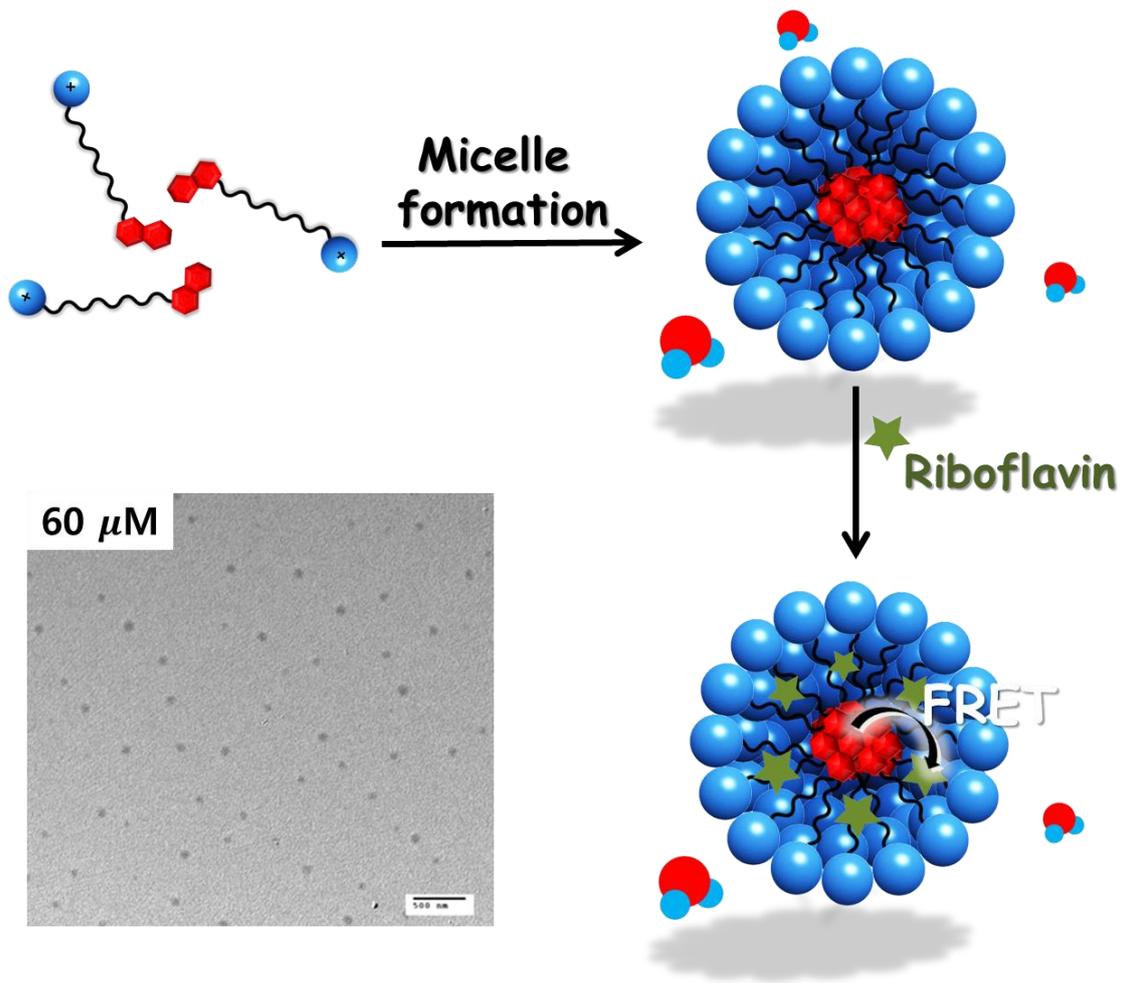
A Highly Sensitive Fluorescent Sensor based on Amplified Quenching in a Conjugated Polyelectrolyte Micelle

Yeonjin Jang, Seoung Ho Lee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

Fluorescence-based assays (FBAs), which are processable in aqueous media, have been explored for use in detection of chemical, biological, radiological, and nuclear agents or elements. However, many FBAs suffer from a low sensitivity that arises from limited sensing transductions for detecting analytes and/or low fluorescence quantum yields induced by reduced excited state energy of fluorophores inherent in aqueous solution. Therefore, the signal amplification for sensing response can provide smart sensory systems for monitoring analytes at very low concentration level. Herein, we demonstrated that self-assembled conjugated polyelectrolyte micelles (CPMs) induces very sensitive signal transduction involving amplified fluorescent changes, which marks a strong difference with the numerous FBAs that have been developed for the sensitive detection. The building block, an amphiphilic coumarin derivative, displays the self-assembled micelle formation in aqueous solution, giving the hydrophobic π -extended conjugated system at the inner part and hydrophilic groups at the periphery. This allows enhanced optical properties, resulting in efficient energy or electron transfer, and high quantum yield. Finally, it is shown that self-assembled CPMs drives highly sensitive detection of Riboflavin at low nanomolar concentrations.



Poster Presentation : **ORGN.P-245**

Organic Chemistry

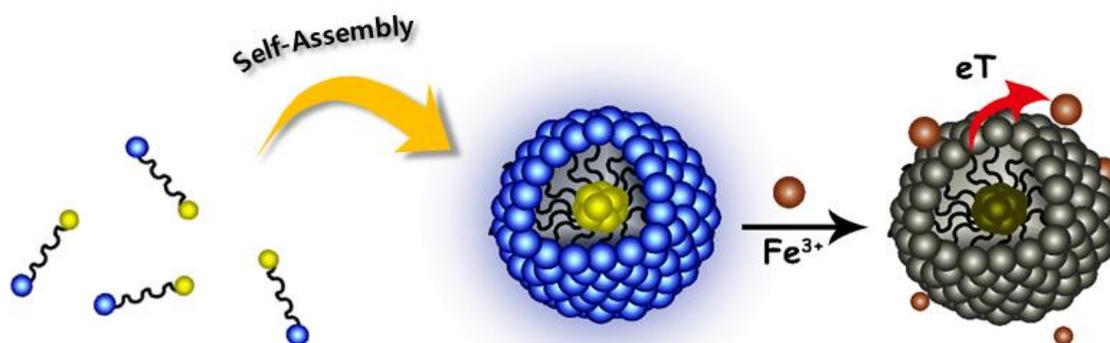
Grand Ballroom, THU 11:00~12:30

A Conjugated Polyelectrolyte Micelle with Strong Fluorescence for Efficient Discrimination of Fe^{2+} and Fe^{3+}

Tae eun Park, Seoung Ho Lee*

Department of Applied Chemistry, Daegu University, Korea

A great effort has been gone into the discrimination of Fe^{2+} and Fe^{3+} ions due to their involvement in various environmental and biological systems. In this work, a conjugated polyelectrolyte micelle based fluorescent approach was developed to discriminate Fe^{2+} and Fe^{3+} based on their induced quenching kinetics. A particular amphiphilic building block with a coumarin moiety and an acetate ionic side chain covalently linked via a hydrophobic alkyl spacer was synthesized. The building blocks display the self-assembled micelle formation in aqueous solution, giving the hydrophobic π -extended conjugated system at the inner part and hydrophilic groups at the periphery. This system allows enhanced optical properties with efficient energy or electron transfer, and high fluorescence quantum yield, which induces amplified quenching in conjugated system of pyrene aggregates in the presence of Fe^{2+} ion.



Poster Presentation : **ORGN.P-246**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

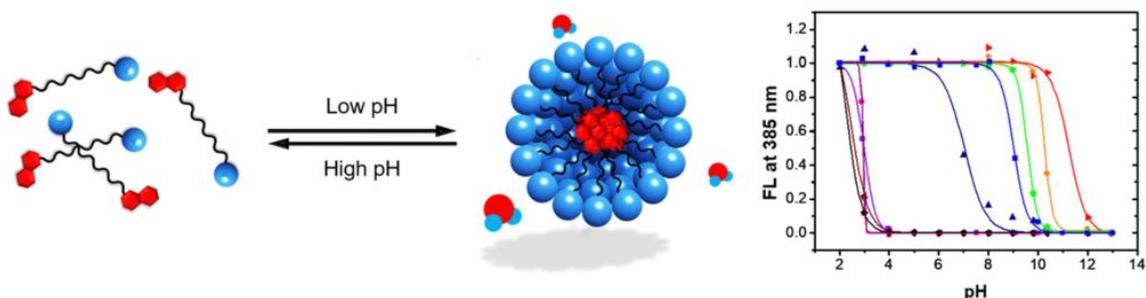
Conjugated Polyelectrolyte Micelles-Based Fluorescent pH Sensors for Broad-Range pH Measurement

Jeongmoo Lee, Seoung Ho Lee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

In this work, effective fluorescent pH sensors have been developed for sensitive and broad-range pH measurement on the basis of conjugated polyelectrolyte micelles (CPMs). Various building blocks, amphiphilic coumarin derivatives, were prepared, in which ionizable amino groups, e.g. aliphatic or aromatic amines, are incorporated as a hydrophilic moiety. These units display the self-assembled micelle formation in wide range of pH, giving the hydrophobic π -extended conjugated system at the inner part and hydrophilic groups at the periphery. This allows enhanced optical properties, resulting in efficient fluorescence intensity changes. To the best of our knowledge, this is the first report the CPM-based fluorescent probes have been used for a wide range of pH detection.



Poster Presentation : **ORGN.P-247**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

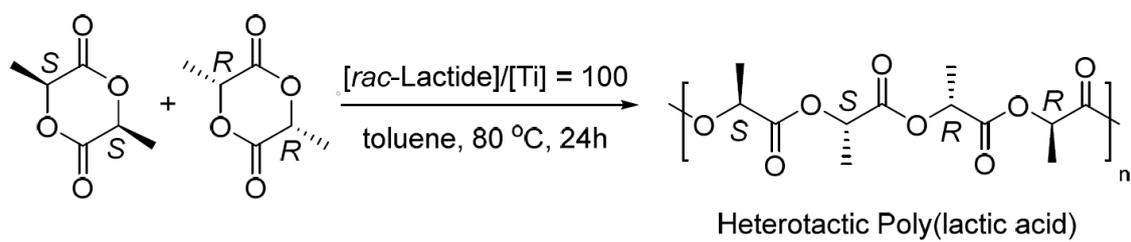
Streocontrolled Ring-Opening Lactide Polymerization with Triaryloxyimino Titanium(IV) Complexes and Computational Analysis of Mechanistic Pathway

Yeo-lib Jeong^{*}, Minjoong Shin¹, Myungeun Seo¹, Kim Hyunwoo^{*}

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

¹Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea

For the last decade, polylactic acid or poly lactide has been one of the most promising ecofriendly, biodegradable products and alternative to petrochemical-based polymers. At the same time, various methods for ring-opening lactide polymerization have been developed with organic, organometallic catalysts. Especially metal complexes attract attention as an effective method to control to get good polymer dispersity (PDI) and selectivity with high reaction speed. In early days, complex with alkali and alkali-earth metals such as Al, Zn, Mg were combined with bidentate ketimine or Schiff base ligands. Group (IV) metal alkoxides like Ti, Zr and Hf increased reactivity and distinct metal effects occurred, connected to much heavier lanthanide and yttrium. For instance, using Hf or Lanthanide under same ligand system usually increased stereoselectivity compared with smaller metal atoms like Al, Ti, etc. We here report a new type of Ti(IV) based catalyst system with iminotris(phenolate) tripodal ligand which is able to control stereoselectivity by simple structure modification. And the origin of stereocontrol by ligand modification was demonstrated through DFT calculation of mechanistic pathway.



Poster Presentation : **ORGN.P-248**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Visible Light Mediated ATRC/ATRP by Phenothiazine Dyes

Geonji Kim, Kyunchan Min, Bongjin Moon*

Department of Chemistry, Sogang University, Korea

Atom transfer radical cyclization (ATRC) is a useful method for formation of ring systems. This reaction can be catalyzed by transition metals such as copper, ruthenium, and nickel. Recently, it has been discovered that such reactions can be also catalyzed by a photo-catalyst under visible-light irradiation at room temperature. Atom transfer radical polymerization (ATRP) is one of the most widely used methods among the reversible deactivation radical polymerization (RDRP) techniques. This method typically employs a redox-sensitive transition metal catalyst to form carbon-carbon bonds transferring halogen atoms. In this study, we have synthesized an organic photo-catalyst based on phenothiazine. We expected strong absorption in the visible light region, reversible single electron transfer and high stability of the radical cation. We then executed visible light-mediated atom transfer radical cyclization (ATRC) of *N*-allyl-*N*-4-tosyl-2-bromo-2,2-dimethylacetamide and visible light-mediated metal free atom transfer radical polymerization (ATRP) of methyl methacrylate using the phenothiazine dye. The ATRP was carried out with methyl-2-bromo methyl propionate as a radical initiator that can be activated by phenothiazine dyes under illumination of blue LED at room temperature. In order to make progress in this polymerization, we suggested that release of free bromide anion disturbed the polymerization and stabilization of the released bromide anion may help the polymerization control. So for this reason, we synthesized cyanostar that might enable to bind bromide anion enhancing its stability.

Poster Presentation : **ORGN.P-249**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

3-Formylindole synthesis using a iodine catalyst

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

Heterocycles are widely used in fields of medicine, chemistry, material chemistry, photochemistry, pesticides, dyes. Among them, indole is easily found in nature and is a molecule with biological activity. Formylindole, which plays an intermediate role in functionalization of indole, is useful in Pharmacology and Biochemistry. Previously, even though several methods for synthesizing 3-formylindole were introduced, toxic substances and environmentally unfavorable reagents, and long reaction times bring about several problems. In this study, an efficient way for C3-formylation is proposed. To explain, the aldehyde group is substituted at the 3-position of the indole by using hexamethylenetetramine as a carbonyl source, iodine as a catalyst, and DMF and H₂O as a solvent. This is advantageous in that no strong acid or metal catalyst is required. In a previous study that only DMF was used as a solvent, a low yield was obtained even after a long reaction time. However, we found that both iodine and HMTA are dissolved in certain ratio of DM F to H₂O. Also, this reaction was proceeded under various conditions. Finally the yield was increased for a short period of time.

Poster Presentation : **ORGN.P-250**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Chiroptical Properties of Chiral Architectures with Triangular Pyramid Shape by the Coassembly of Helical Peptides

Jae-Hoon Eom, Jintaek Gong¹, Rokam Jeong, Hee-Seung Lee*

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

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

Chiroptical properties are very important for optical applications such as the implementation of metamaterials at the molecular level as well as the supramolecular level. Our group recently reported various foldectures which have very uniform and well-defined 3D architectures by the self-assembly of artificial peptides with simple and rigid scaffolds. Foldectures have the advantage to easily achieve supramolecular chirality by controlling the chirality at the molecular level. However, the foldectures studied so far are composed of a simple homogeneous foldamer of eleven or twelve helical types. In the biological system, the 3D complex protein architecture is created through the various interactions of subunits with a variety of compositions and structures. To better understand the intermolecular interaction between different subunit components, it is necessary to study the coassembly mixed with various peptides. Coassembly is powerful and facile way to implement more complex and new molecular architecture for biomolecules or engineering materials. Herein we report new chiral foldectures which have triangular pyramid shapes by the coassembly of 11-helical foldamers. Foldamer packing motif was revealed by X-ray diffraction method, that provides an important structural information for intermolecular interactions. In addition, we have demonstrated new chiroptical properties through the diverse experimental methods. Our research proves useful in designing new strategies for desired complex architectures with functional groups.

Poster Presentation : **ORGN.P-251**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

A new method for the synthesis of benzisothiazolone derivatives in one step reaction

Seongjeong Lee, Dong wook Kang^{1,*}

Department of Pharmaceutical Science and Technology, Daegu Catholic University, Korea

¹*Department of Pharmaceutical Science and Technology, Daegu Catholic University, Korea*

This study is a methodological study on the synthesis of benzisothiazolone derivatives as potential anticancer agents. Conventional benzisothiazolone synthesis methods yield products in three to five reaction steps, but the new method is more efficient because it can obtain products in one step reaction. A new method for the synthesis of benzisothiazolone uses 2,2'-dithiodibenzoic acid and various amine compounds as starting materials. Under a certain reaction condition, the amide coupling reaction proceeds through the diamide compound to the benzisothiazolone. However, depending on the electronic environment of the amine compound used in the reaction, the yield of amide intermediate is increased and the yield of benzisothiazolone is lowered. In order to improve the low yield, it is possible to obtain the product of improved yield by incorporating benzenethiolate after the reaction by using iodine. Benzisothiazolone compounds are well known as histone acetyltransferases inhibitors and can be developed as potential anticancer agents.

Poster Presentation : **ORGN.P-252**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of quercetin mono-gallate conjugates with therapeutic effects similar to EGCG

Jongyun Jang, Dong wook Kang^{1,*}

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Epigallocatechin gallate(EGCG), a kind of flavonoids contained in green tea, has the effect of inhibiting the expression of EZH2 and preventing Alzheimer's disease. Inhibition of H₂O₂ induced apoptosis through regulation of Bcl-2 and Bax expression in ROS signaling associated with apoptosis in endothelial cells. It is known to be about 100 times more effective than Tamiflu, a treatment for swine flu. However, EGCG can cause severe liver toxicity if the daily intake is over 800 mg, making it difficult to develop therapeutic agents. This study relates to a method for synthesizing a quercetin mono-gallate conjugate compound, which has a structure similar to EGCG with a therapeutic effect of various diseases and has a low toxicity. It is discussed the synthesis of four quercetin mono-gallate conjugates. The process of conjugating a gallic acid at the 4'-hydroxyl group of quercetin is as follows. 3', 4'-hydroxyl groups are protected with acetal ring structure using dichlorodiphenylmethane and then 3-,7-hydroxyl groups are protected by benzylation. Continuously, 3', 4'-acetal ring is deprotected and then, acetylation proceeds to the 4'-hydroxyl group, and the benzylation is carried out to protect the 3'-hydroxyl group. Acetyl group of the 4'-position is hydrolyzed during the benzylation of the 3'-hydroxyl group. Finally, the 4'-hydroxyl group of quercetin is coupled with tribenzyl-gallic acid, and all benzyloxy groups are deprotected through a hydrogenation reaction. The remaining quercetin mono-gallate coupling compounds are prepared in a similar procedure.

Poster Presentation : **ORGN.P-253**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and photophysical study of 2-fluorenyl-1,2,3-triazole-labeled 2'-deoxyuridine, 2'-deoxyadenosine, 2'-deoxyguanosine, 2'-deoxycytidine, and their oligonucleotides

SeungWoo Hong, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

Fluorene is a useful fluorophore because it has a good quantum yield and is less bulky than other commonly used fluorophore. Therefore we previously synthesized fluorene labeled 2'-deoxyuridine (U^{FL}) through an ethynyl linker and observed good solvent dependent photophysical properties. In this study, we have synthesized triazole-linked fluorenyl 2'-deoxyuridine (U^{FT}), 2'-deoxyadenosine (A^{FT}), 2'-deoxyguanosine (G^{FT}), 2'-deoxycytidine (C^{FT}) through copper catalyzed azide-alkyne cycloaddition (CuAAC). All four modified nucleosides displayed different fluorescence intensities and emission maxima in different solvents, indicating its potential for application as an environmentally sensitive probe. In addition, we inserted U^{FT} , A^{FT} , G^{FT} , and C^{FT} at the central position of an oligonucleotides (ODNs). Herein the photophysical properties of fluorene-labeled nucleosides with a triazole linker and their corresponding ODNs will be discussed.

Poster Presentation : **ORGN.P-254**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Supramolecular complexes for organic hybrid thermoelectric materials with high Seebeck coefficient and low thermal conductivity

JaeGyu Jang, Sung Hyun Kim^{1,*}, Jong-in Hong*

Division of Chemistry, Seoul National University, Korea

¹Carbon Convergence Engineering, Wonkwang University, Korea

We report on supramolecular complexes of amphiphilic molecules and a single-wall carbon nanotube as thermoelectric hybrid materials. A hybrid material based on an amphiphilic molecule having the alkyl chain on the aromatic core exhibited higher ZT value compared to a hybrid material formed from amphiphiles without the alkyl chain through de-bundled SWNTs, more densely adsorbed amphiphiles on the SWNT surface, and induced phonon scattering. In addition, the optimization of length and thickness of supramolecular structures further improve the TE performance of hybrid materials. The details will be explained in the presentation.

Poster Presentation : **ORGN.P-255**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of novel biaryl sulfate core based hepatitis C virus NS5A inhibitors using sulfur(VI) fluoride exchange reaction

Youngsu You, Byeong Moon Kim*

Division of Chemistry, Seoul National University, Korea

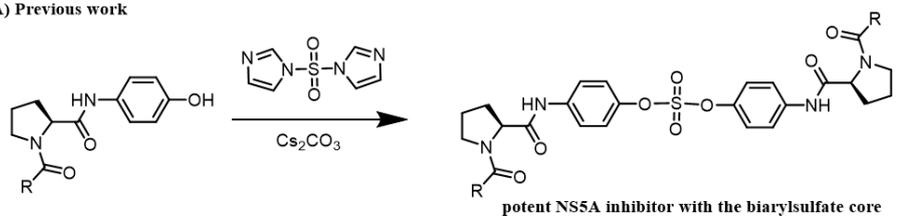
A chemoselective coupling reaction between an arylsulfonyl fluoride and an aryl silyl ether is known as the sulfur(VI) fluoride exchange (SuFEx) reaction. This “sulfate click reaction” is extremely efficient and provides the desired products in essentially quantitative yields.

Our laboratory recently reported the discovery of biaryl sulfate core-based HCV NS5A inhibitors, which exhibit two-digit picomolar EC₅₀ values against HCV genotype 1b and 2a. Herein, we demonstrate the utilization of the SuFEx chemistry to modify the structures of sulfate-core part of the NS5A inhibitors for further optimization of antiviral activities against HCV. The products obtained through the SuFEx click reactions were obtained in high yields. Among the compounds prepared through the SuFEx chemistry, products with potent NS5A inhibitors had two-digit picomolar EC₅₀ values against GT-1b and single digit nanomolar activities against GT-2a strain of HCV. In addition, the biotinylated probe targeting NS5A protein and nonsymmetrical inhibitors containing an imidazole and amide linkers at the opposite sides of the core sulfate structures were also synthesized through the use of the same synthetic methodology.

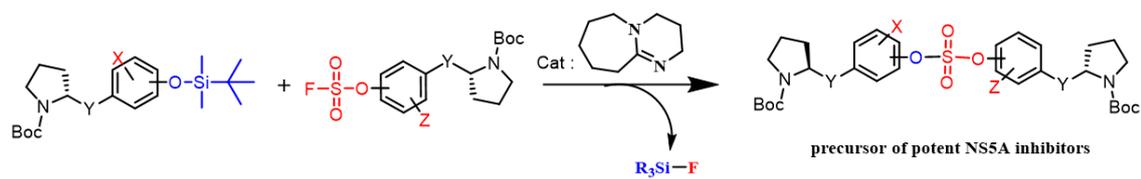
Reference

1. You, Y. S.; Kim, H. S.; Bae, I. H.; Lee S. Gi.; Jee M. H.; Keum G. C.; Jang S. K.; Kim B. M., *Eur. J. Med. Chem.*, **2017**, 125, 87.
2. Bae, I. H.; Kim, H. S.; You, Y. S.; Chough, C.; Choe, W.; Seon, M. K.; Lee, S. G.; Keum, G.; Jang, S. K.; Kim, B. M., *Eur. J. Med. Chem.*, **2015**, 101, 163.
3. Bae, I. H.; Choi, J. K.; Chough, C.; Keum, S. J.; Kim, H.; Jang, S. K.; Kim, B. M., *ACS Med. Chem. Lett.*, **2014**, 5 (3), 255.

(A) Previous work



(C) This work
(Synthesis of NSA inhibitors using the SuFEx chemistry)



Poster Presentation : **ORGN.P-256**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

S-thiotrialkylsilyl cysteines: Novel persulfide precursors for exploring of cysteine posttranslational modifications

Yu Rim Kwon, Sol Ryeong Im¹, Chung-Min Park^{2,*}

Department of Chemistry, Gangneung-Wonju National University, Korea

¹*Department of Chemical Advanced Materials, Gangneung-Wonju National University, Korea*

²*Chemical Advanced Materials, Gangneung-Wonju National University, Korea*

Persulfides (RSSH) have been known as important components along with hydrogen sulfide (H₂S) and hydrogen polysulfides (H₂Sⁿ) in sulfur-mediated redox cycles and involve in cell signaling. However, the study of persulfide chemistry remains a challenge because of the lability of the RSSH compounds and a lack of efficient precursors. Reported here is the synthesis and evaluation of S-thiotrialkylsilyl (R'SSSiR₃) compounds as potential persulfide precursors. The compounds are moisture-stable and undergo desilylation with fluoride ions to release of the corresponding persulfides. In addition, we will discuss that pH-dependent hydrolytic removal of various silyl groups on the persulfide precursors releases the corresponding persulfides in control fashion.

Poster Presentation : **ORGN.P-257**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Facile and rapid synthesis of dehydroalanines from S-thioalkylsilyl cysteines

Sol Ryeong Im, Yu Rim Kwon¹, Chung-Min Park^{2,*}

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²*Chemical Advanced Materials, Gangneung-Wonju National University, Korea*

The α,β -unsaturated amino acids (dehydroalanines) are found in a variety of biological peptides and natural products. Synthetically, they can be versatile precursors to unnatural amino acids which can be used to alter the structural properties of peptides. The synthesis of dehydroalanines has previously been achieved by many different methods. However, most procedures are not selective or are incompatible with other amino acid residues in the peptide or require many steps and long reaction time. Reported in this work is the rapid synthesis of dehydroalanines from S-thioalkylsilyl cysteine derivatives under mild reaction conditions. The cysteine residue in peptides can be easily functionalized to S-thioalkylsilyl moiety and they are subsequently and conveniently converted into the corresponding dehydroalanines at the desired position.

Poster Presentation : **ORGN.P-258**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Selective sensor for mercury ions with tryptophan based fluorophore

Jaewook Jeong, Keun Hyeung Lee^{1,*}

Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

The sensitive detection and quantification of transition heavy metal ions are highly important because they play important roles in body system and also have toxicity on the environment. Mercury ions, among the transition heavy metal ions, are one of the most toxic metal ions in human body. For that reason, various types of detectors have been developed for mercury ions and also chemosensors. Among the detectors, chemosensors have a superiority in sensitivity and effective analytical way. Herein, we developed a series of fluorescence sensors based on NBD as a fluorophore and tryptophan as a receptor connected with different length of glycine chains for detection of mercury ions. These sensors detect mercury ions selectively either by turn on or turn on response depending on the length of linkers between the NBD and the tryptophan part.

Poster Presentation : **ORGN.P-259**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Ratiometric Fluorescent Detection of Indium(III) with High Selectivity and Sensitivity by a Fluorescent Probe Containing Phosphoserine as a Receptor

Mehta Pramod Kumar, Keun Hyeung Lee^{1,*}

Department of Chemistry & Chemical Engineering Con, Inha University, Korea

¹Department of Chemistry, Inha University, Korea

Indium is one of the most widely used scarce metals for manufacturing various electronic devices including notebooks, mobile phones, and PC monitors. Recent studies revealed that indium and its compound could cause several toxicities to human beings and animals. However, there is no report about ratiometric fluorescent detection of In(III) in aqueous solutions. We synthesized a fluorescent probe (1) for In(III) based on a phosphoserine as a receptor with a pyrene fluorophore using solid phase synthesis. 1 showed highly sensitive ratiometric response to In(III) in purely aqueous solutions by increasing excimer emission intensity at 476 nm with a concomitant decrease in monomer emission intensity at 395 nm. 1 showed sensitive ratiometric responses to In(III) over a wide range of pH (2 < pH

Poster Presentation : **ORGN.P-260**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Foldectures from the Self-Assembly of Chimeric Foldamers

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

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

Nature builds incredibly complex, functional systems. The design of the building block is very important to understand the formation mechanism of the complex structure. Self-assembly of micro-sized architectures has the potential to provide the basis for new technology. We used octameric foldamers composed of 2-aminoisobutyric acid (Aib) and α -amino acid (trans-2-aminocyclopentane carboxylic acid, ACPC) in a 1:1-alternating β -peptide foldamer. These foldamers are reported to display two helical conformations, the 11-helix and the 14/15-helix. This phenomenon is similar to structural changes with the 310-helix and α -helix in natural proteins. The intermediate of structural changes can be understood through self-assembly. Our group recently reported various foldectures which have highly homogeneous and unique 3D morphologies derived from the self-assembly of foldamers. To understand the correlation between the helical type and the 3-dimensional structure, it is necessary to study the foldamers with chimeric helical types. Herein we report a new foldecture which has a concave-faced cuboid shape by the self-assembly of chimeric foldamer of 11-and 14/15-helix. Foldamer packing structure was resolved by powder X-ray diffraction (PXRD) analysis and provides important structure information for the unusual 3D architecture. This study will play an important role in designing complex 3D architecture analogous to proteins.

Poster Presentation : **ORGN.P-261**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

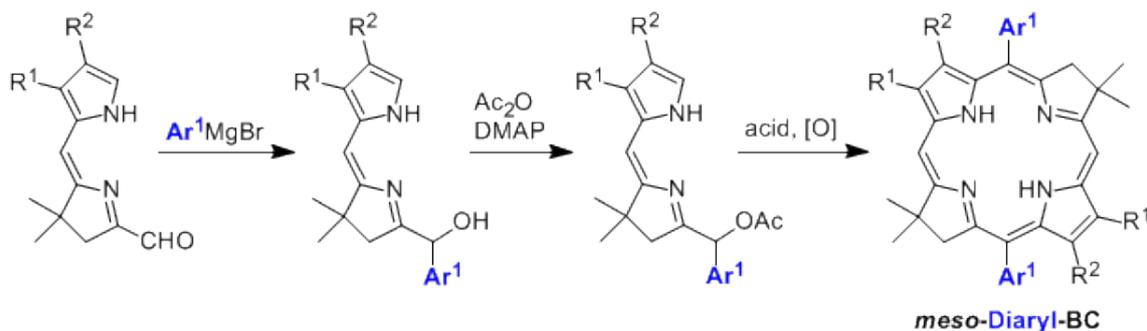
Synthesis of Meso-Diaryl-Bacteriochlorins: Characterization and Absorption Spectral Properties

Han-Je Kim^{*}, Jonathan Lindsey¹

General Science Education, Gongju National University of Education, Korea

¹Department of Chemistry, North Carolina State University, United States

Synthetic bacteriochlorins are attractive for diverse photochemical studies. meso-Diarylbacteriochlorins were prepared by the self-condensation of dihydrodipyrin–acetates following an Eastern-Western (E-W) joining process. The bacteriochlorins bear a gem-dimethyl group in each pyrroline ring to ensure stability toward oxidation. Treatment of a known 3,3-dimethyldihydrodipyrin-1-carboxaldehyde with an aryl Grignard reagent afforded the dihydrodipyrin-1-(aryl)carbinol, and upon subsequent acetylation, the corresponding dihydrodipyrin-1-methyl acetate (dihydrodipyrin–acetate). Self-condensation of the dihydrodipyrin–acetate gave a meso-diarylbacteriochlorin (E-W route). The aromatization process entails a $2e^-/2H^+$ (aerobic) dehydrogenative oxidation following the dihydrodipyrin self-condensation. The bacteriochlorins exhibit characteristic bacteriochlorophyll-like absorption spectra, including a Qy band in the region 726–743 nm. In this poster, synthesis, characterization, and absorption spectral properties of the meso-diaryl-bacteriochlorins will be described.



Poster Presentation : **ORGN.P-262**

Organic Chemistry

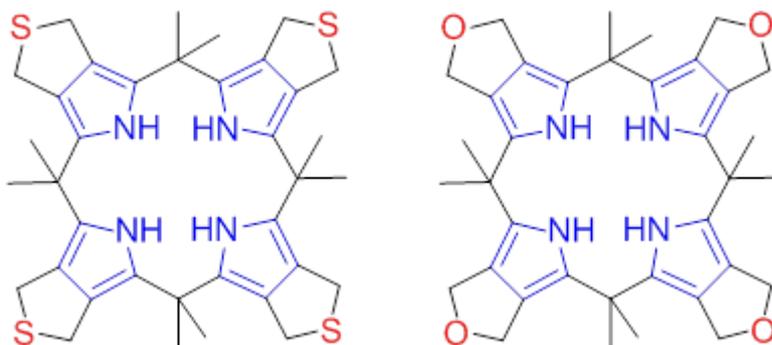
Grand Ballroom, THU 11:00~12:30

Synthesis and ion-pair recognition property of thiophene- or furan-fused calix[4]pyrroles

Hyun Seong Kang, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

Selective recognition of ion-pair has drawn great attentions due to their applications in medicinal and environmental chemistry. The designing and synthesizing ion-pair receptors possessing high selectivity is highly desirable in conjunction with the development of real chemosensors. Among those receptors, calix[4]pyrroles are well known to be efficient receptors for various anionic species and ion-pair in some cases. Variety of modification of the parent macrocycle have been developed for the last ten years. Those modifications are generally focused on either the β -pyrrolic positions or the meso-positions. Usually introduction of electron donating substituents at β -pyrrolic positions decreases the anion binding affinity because weakened hydrogen bonding and destabilizing steric interactions incurred upon anion binding. Here, we report novel ion-pair receptors bearing functionalities that can recognize both cations and anions with high affinity and selectivity. The ion-pair binding properties of the synthesized receptors will be presented in detail.



Poster Presentation : **ORGN.P-263**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Spectroscopic Investigation of Perylene-Containing Diimides

Sung Sik Kim

Department of Chemistry, Chonbuk National University, Korea

Several types of diimides were synthesized and their structures were investigated by NMR and other spectroscopic data. Perylenediimide trimers were prepared starting from perylene dianhydride. Dialkyl groups were introduced to the aromatic moiety in the final compounds. As for benzene rings linked with perylene moiety, t-butyl groups were also introduced to increase the solubility in organic solvents. Perylene dianhydride was converted into diimide derivative. Diimide was converted into the corresponding anhydride imide. Reaction of the intermediate with 1,3,5-benzenetriamine (BTA) yielded the second target compound. BTA was used right after preparing from 3,5-dinitroaniline. Perylene anhydride imide was added to BTA to give a diamine intermediate, which was reacted with excess perylene anhydride imide to yield the target molecule. The final step was carried out with imidazole and zinc acetate. Another target molecule having 2,6-diisopropyl benzene ring and t-butyl phenoxy group was also synthesized.

Poster Presentation : **ORGN.P-264**

Organic Chemistry

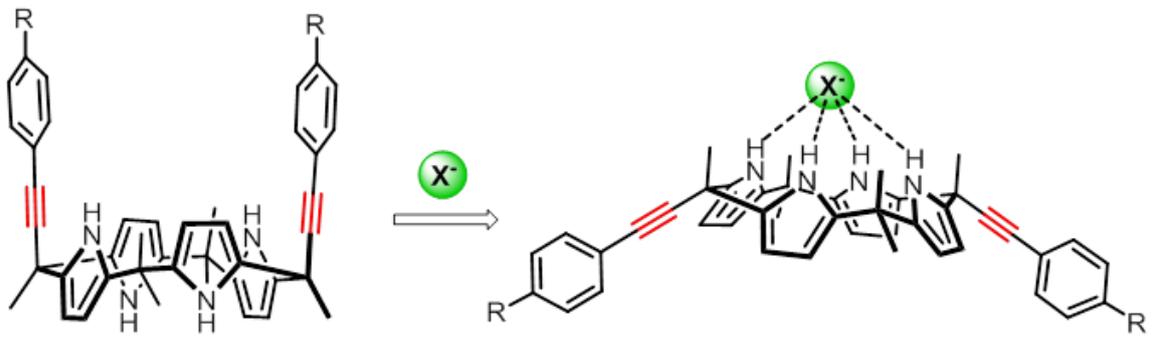
Grand Ballroom, THU 11:00~12:30

meso-Substituents effects on the anion binding affinities and complex conformations of calix[4]pyrroles: A case study with meso-bis-arylethynyl calix[4]pyrroles

Ranjan Dutta, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

Functionalization of meso-positions of calix[4]pyrroles is the most viable strategy to develop topologically new receptors with tunable guest binding properties. In recent years, meso-aryl calix[4]pyrroles have been extensively studied as effective receptors for anions, ion-pairs and transmembrane anion transporters where the electronic natures of meso-substituents play crucial roles.¹ Meso-aryl calix[4]pyrroles usually adopted cone conformation during anion complexation and anion binding occurred in between the axially positioned meso-aryl groups. This trend of pocket side binding of anion persist even in cases of meso-tetra-aryl and meso-tetra-alkyl calix[4]pyrroles during anion complexation. We have designed and synthesized a series of meso-bis-arylethynyl calix[4]pyrroles by directly anchoring ethynyl groups at the diametrical opposed meso-positions.² These alkynyl extended calix[4]pyrroles are established as superior halide anion receptors to their analogous meso-aryl congeners. Single crystal X-ray structure analysis and solution state binding studies of the halide–host complexes demonstrate a pseudo-equatorial alignment of the meso-arylethynyl groups, which are unprecedented and quite different from the meso-aryl calix[4]pyrroles reported thus far. Comparative studies on effects of meso-substituents toward anion binding affinity, host-guest geometry are presented in cases of these meso-ethynyl extended systems.



Poster Presentation : **ORGN.P-265**

Organic Chemistry

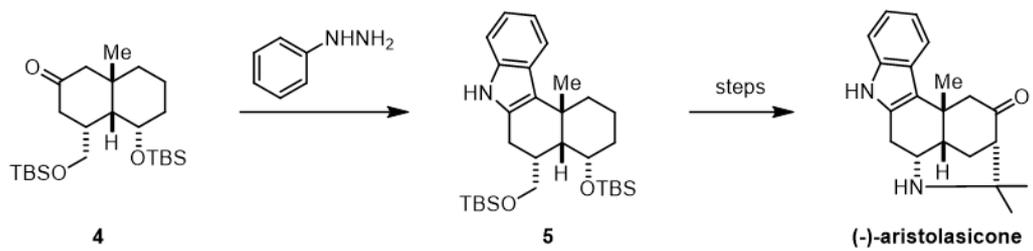
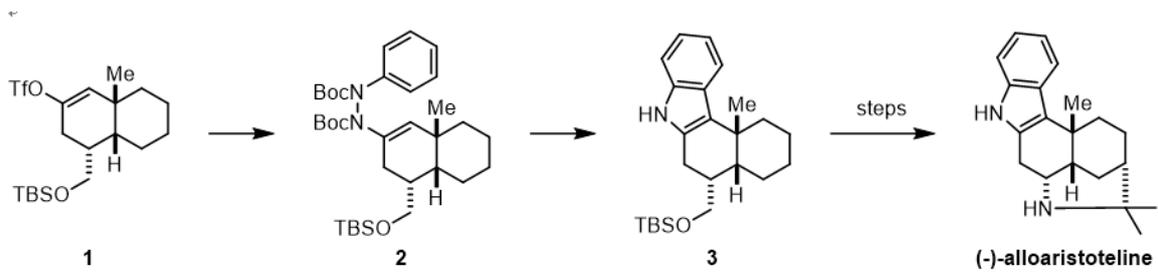
Grand Ballroom, THU 11:00~12:30

Total Syntheses of (-)-Alloaristoteline and (-)-Aristolasicone

Tae-Hong Jeon, Jang Yeop Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Abstract In our recent report, we have demonstrated that ene-hydrazide prepared from enol triflate in regiochemically defined form may undergo Fischer indolization with no regiochemical scrambling.¹ Applying to this method, we recently reported total syntheses of (+)-aspidospermidine and (-)-tabersonine.² As a part of our ongoing study for application of this method to the synthesis of natural products, we designed synthetic routes toward the total syntheses of aristotelia alkaloids, (-)-alloaristoteline and (-)-aristolasicone. We began the synthetic exploration by preparing enol triflate **1** from the corresponding enone via a Michael addition using Me₂CuLi followed by in-situ triflation. Subsequent C-N coupling with phenyl hydrazide afforded the key ene-hydrazide **2**. Regioselective Fischer indolization under Lewis acidic conditions furnished indole **3** pertaining a cis-fused decalin core of (-)-alloaristoteline. During the study, we observed a unexpected regiochemical control when cis-2-decalone **4** was subjected to the classical Fischer indolization. The origin of the regioselectivity as well as our progress in the total syntheses of (-)-alloaristoteline and (-)-aristolasicone will be discussed.**References** 1. Lim, B.-Y.; Jung, B.-E.; Cho, C.-G. *Org. Lett.* **2014**, 16, 4492. 2. Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.* **2017**, 19, 6168-6171.



Poster Presentation : **ORGN.P-266**

Organic Chemistry

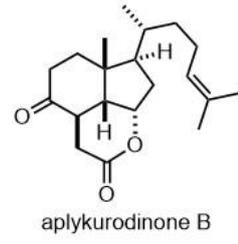
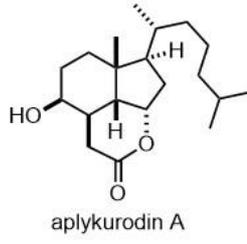
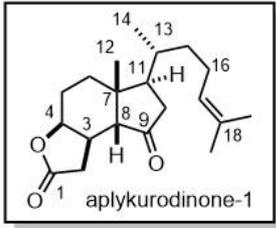
Grand Ballroom, THU 11:00~12:30

Internal H-bonding mediated efficient stereo-, regio-selective intramolecular Diels-Alder reaction of 2-pyrone and formal synthesis of (+)-aplykurodinone-1

Joon Ho Lee, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Aplykurodines are steroids natural products which have tricyclic ring core with various biological activities including cytotoxicity against a range of human cancer cells. Aplykurodinone-1 whose structure is shown below has gained much interest for the unusual cis-fused hydrindane core decorated with six contiguous stereocenters, also found in other aplykurodines, and C11 side chain presenting C20 issue in steroid synthesis.¹As a part of our ongoing study on 3,5-dibromo-2-pyrone toward target oriented synthesis,² we have devised a new synthetic route to (+)-aplykurodinone-1 by way of internal hydrogen bonding mediated asymmetric intramolecular Diels-Alder reaction. This elaborated 2-pyrone IMDA reaction turned out to proceed in perfect π -facial and endo selectivity, providing the cis-hydrindane core as well as all substituents with right stereochemistry necessary for the synthesis of aplykurodinone-1. Transformations including hydrogenation, lactone ring formation and elimination gave the Danishefsky's intermediate as a formal synthesis of (+)-aplykurodinone-1. **Reference** 1. (a) Spinella, A.; Gavagnin, M.; Crispino, A.; Cimino, G.; Martinez, E.; Ortea, J.; Sodano, G. *J. Nat. Prod.* 1992, 55, 989–993. (b) Miyamoto, T.; Higuchi, R.; Komori, T. *Tetrahedron Lett.* 1986, 27, 1153–1156. (c) Gavagnin, M.; Carbone, M.; Nappo, M.; Mollo, E.; Roussis, V.; Cimino, G. *Tetrahedron* 2005, 61, 617–621. 2. (a) Jung, Y.-G.; Kang, H.-U.; Cho, H.-K.; Cho, C.-G. *Org. Lett.* 2011, 13, 5890. (b) Jung, Y.-G.; Lee, S.-C.; Cho, H.-K.; Nitin B. D.; Song, J.-Y.; Cho, C.-G. *Org. Lett.* 2013, 15, 132. (c) Cho, H.-K.; Lim, H.-Y.; Cho, C.-G. *Org. Lett.* 2013, 15, 5806. (d) Shin, H.-S.; Jung, Y.-G.; Cho, H.-K.; Park, Y.-G.; Cho, C.-G. *Org. Lett.* 2014, 16, 5718.



Poster Presentation : **ORGN.P-267**

Organic Chemistry

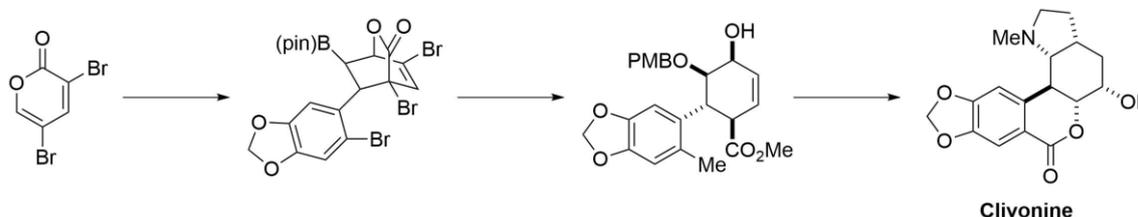
Grand Ballroom, THU 11:00~12:30

Total synthesis of (\pm)- Clivonine via Cycloaddition with 3,5-Dibromo-2-pyrone

Cheng-Dong Wang, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Diels-Alder reaction of 2-pyrone can be exceptionally powerful for the synthesis of structurally complex natural products, constructing multiple carbon-carbon bonds in a single operation¹. As a part of our ongoing study exploring the utility of 3,5-dibromo-2-pyrone in target-oriented synthesis², we have further envisioned that the aforementioned synthetic strategy could be also effective for clivonine a lycorenine-type amaryllidaceae alkaloid isolated from *Clivia miniata* Regel in 1956. Our recently achieved end-game synthesis of this natural product will be presented. 1.a) Chung, S. I.; Seo, J. B.; Cho, C.-G. *J. Org. Chem.* 2006, 71, 6701. b) Shin, J. T.; Hong, S. H.; Shin, S. H.; Cho, C.-G. *Org. Lett.* 2006, 8, 3339. 2.(a) Chang, J. H.; Kang, H.-U.; Jung, I.-H.; Cho, C.-G. *Org. Lett.* 2010, 12, 2016. (b) Tam, N. T.; Jung, E.-J.; Cho, C.-G. *Org. Lett.* 2010, 12, 2012. (c) Tam, N. T.; Cho, C.-G. *Org. Lett.* 2008, 10, 601. (d) Tam, N. T.; Chang, J.; Jung, E.-J.; Cho, C.-G. *J. Org. Chem.* 2008, 73, 6258. (e) Shin, I.-J.; Choi, E.-S.; Cho, C.-G. *Angew. Chem., Int. Ed.* 2007, 46, 2303. (f) Tam, N. T.; Cho, C.-G. *Org. Lett.* 2007, 9, 3319. (g) Kim, H.-Y.; Cho, C.-G. *Prog. Heterocycl. Chem.* 2007, 18, 1. (h) Ryu, K.; Cho, Y.-S.; Cho, C.-G. *Org. Lett.* 2006, 8, 3343.



Poster Presentation : **ORGN.P-268**

Organic Chemistry

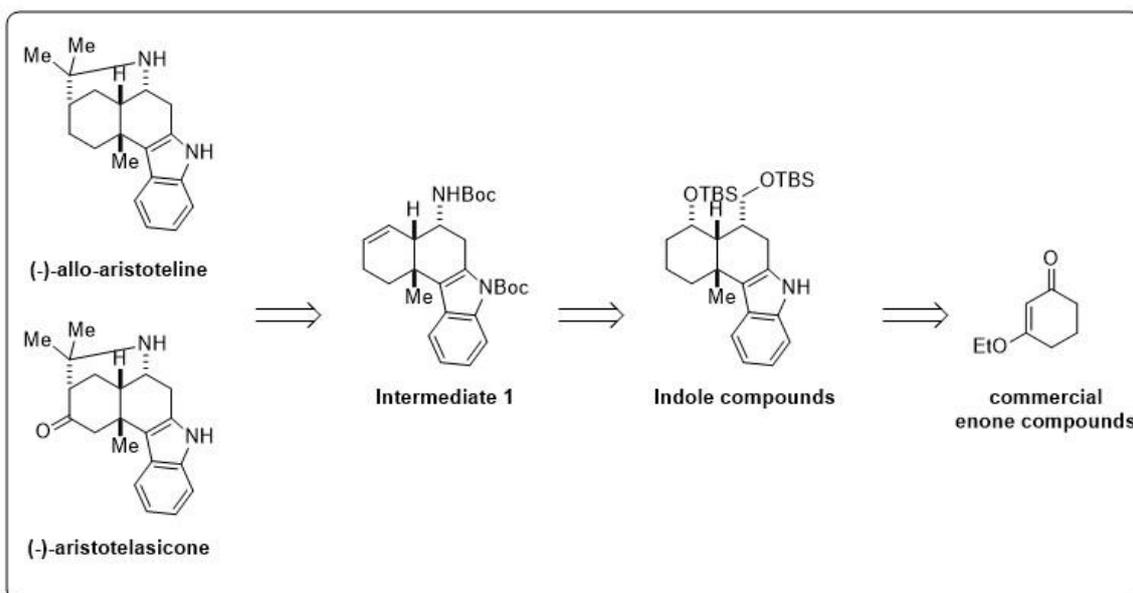
Grand Ballroom, THU 11:00~12:30

Total synthesis of aristotelia alkaloids via unexpected regioselectivity in fischer indolization

Jang yeop Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Abstract As a part of our ongoing study about regioselective fischer indolization, we planned to synthesize aristotelia alkaloids which has penta-cyclic core. To demonstrate the efficiency of our method, we conducted a comparative experiment between conventional fischer indolization and our lab's fischer indolization method. Interestingly, there is a perfect regioselectivity in desired indole compounds with conventional fischer indolization conditions. With enough amount of indole compounds in hands, we could synthesize desired key intermediate 1 with several functional group transformation. we are struggling to synthesize (-)-allo-aristoteline and (-)-aristolasicone from key intermediate 1. Reference 1. (a) Lim, B.-Y.; Jung, B.-E.; Cho, C.-G. *Org. Lett.* 2014, 16, 4492. (b) Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.* 2017, 19, 6168-6171.



Poster Presentation : **ORGN.P-269**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

PdPt–Fe₃O₄ NPs catalyzed one pot, chemoselective synthesis of unsymmetrical secondary amines from benzonitrile and nitroalkanes

Jin hee Cho, Sangmoon Byun¹, Ahra Cho¹, Byeong Moon Kim^{1,*}

Seoul National University, Korea

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

We have reported successful catalytic nitro-reduction and arylsilylation using bimetallic PdPt–Fe₃O₄ Nps, which are heterodimeric magnetically recyclable nanocatalysts. This bimetallic PdPt–Fe₃O₄ catalysts show a great possibility to become a promising tool for a wide range of scientific and industrial application with high efficiency, sustainability and environment-friendliness. Herein, we report a new synthetic strategy for one-pot selective synthesis of secondary amines via reductive amination of nitriles with nitroalkanes using the PdPt-Fe₃O₄ catalysts. The reactions involving the catalysts are very efficient for one-pot cascade hydrogenation of a nitroalkanes and the reductive alkylation of the resulting amines with an imine generated in situ from benzonitrile from the same catalysts. This method allows for highly chemoselective synthesis of unsymmetrical secondary amines with the advantage of avoiding the use of alkyl halides and/or carbonyl compounds. Also, direct use of benzonitrile and nitroalkanes offer a green strategy for the preparation of amines, which are important building blocks for pharmaceutical, agrochemical and biotechnology applications

Poster Presentation : **ORGN.P-270**

Organic Chemistry

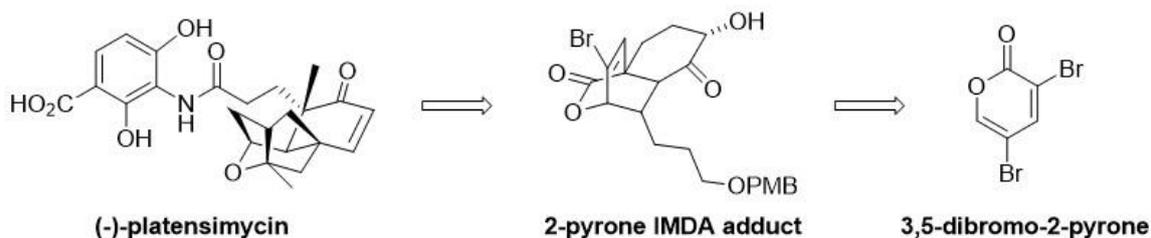
Grand Ballroom, THU 11:00~12:30

Study for total synthesis of (-)-platensimycin by Intramolecular Diels-Alder of 2-pyrone

Hyo-mi Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

We have investigated 3,5-dibromo-2-pyrone towards target-oriented synthesis, utilizing its peculiar reactivity as a neutral diene and the selective maneuverability of the two bromine groups. Such efforts have allowed syntheses of a serious bioactive natural products. Inspired by our recent success on internal hydrogen bonding mediated asymmetric Diels-Alder reaction, we have launched a program inventing a new synthetic strategy to (-)-platensimycin. Included in the new route are C3-selective Stille-coupling reaction of 3,5-dibromo-2-pyrone, chemo-selective hydrogenation and intramolecular Diels-Alder cyclization. Presented herein is our recent progress toward total synthesis of (-)-platensimycin. **Reference 1.** (a) Kim, W.-S.; Kim, H.-J.; Cho, C.-G. *J. Am. Chem. Soc.* **2003**, *125*, 14288. (b) Tam, N. T.; Cho, C.-G. *Org. Lett.* **2007**, *9*, 3391. (c) Shin, I.-J.; Choi, E.-S.; Cho, C.-G. *Angew. Chem. Int. Ed.* **2007**, *46*, 2303. (d) Chang, J. H.; Kang, H.-U.; Jung, I.-H.; Cho, C.-G. *Org. Lett.* **2010**, *12*, 2016. (e) Jung, Y.-G.; Kang, H.-U.; Cho, H.-K.; Cho, C.-G. *Org. Lett.* **2011**, *13*, 5890. (f) Jung, Y.-G.; Lee, S.-C.; Cho, H.-K.; Nitin B. D.; Song, J.-Y.; Cho, C.-G. *Org. Lett.* **2013**, *15*, 132. (g) Cho, H.-K.; Lim, H.-Y.; Cho, C.-G. *Org. Lett.* **2013**, *15*, 5806. (h) Shin, H.-S.; Jung, Y.-G.; Cho, H.-K.; Park, Y.-G.; Cho, C.-G. *Org. Lett.* **2014**, *16*, 5718.



Poster Presentation : **ORGN.P-271**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

One-pot oxidative esterification of 5-hydroxymethylfurfural into furan-2,5-dimethylcarboxylate using alloy AuPd-Fe₃O₄

Ahra Cho, Sangmoon Byun, Jin Hee Cho, Byeong Moon Kim*

Division of Chemistry, Seoul National University, Korea

Exploring heterogeneous catalysis for transforming sustainable biomass into high value-added intermediates or chemicals is of significant importance. The development of catalysts for the conversion of 5-hydroxymethylfurfural (HMF) into high value-added 2,5-furandicarboxylic acid (FDCA) that can form polyethylene furanoate (PEF) has been established. However, furan-2,5-dimethylcarboxylate (FDMC) has more advantages as a monomer because of its higher solubility than FDCA, which has poor solubility in most solvents. In addition, it is important to be able to show catalytic activity at mild conditions to recycle expensive noble metals in chemical industry. To our best knowledge, a catalyst capable of converting HMF to FDMC at room temperature under 1 atm O₂ has not been reported. Herein, we report high-performance bimetallic alloy AuPd-Fe₃O₄ catalyst, which exhibits high efficiency in the synthesis of furan-2,5-dimethylcarboxylate (FDMC) through one-pot oxidative esterification from 5-hydroxymethylfurfural (HMF) at r.t. under atmospheric pressure of O₂. Compared with individual reactions employing either of the monometallic catalysts, the alloy AuPd-Fe₃O₄ nanoparticles (NPs) exhibited synergy effect, showing unprecedented catalytic activity. Also, 1:1 Au/Pd ratio was found to be the best combination for the highest FDMC yield. Interestingly, monometallic Au-Fe₃O₄ catalyst showed high yield and selectivity for the synthesis of 5-hydroxymethyl furoic acid methyl ester (HMFE). The magnetically recyclable AuPd-Fe₃O₄ NPs were readily recycled and reused three times using an external magnet, and the particles showed no significant change in morphology after recycle.

Poster Presentation : **ORGN.P-272**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and fluorescence property analysis of 2'-deoxyuridines labeled with fluorene directly or diacetylenyl linker and their corresponding oligonucleotides

So Young Lee, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

Fluorescent nucleoside analogs that are sensitive to their local environment, demonstrating changes in the fluorescent properties when induced by changes in polarity, pH, or even structure, have become powerful tools for the investigation of nucleic acid structure, dynamics, and recognition. Therefore we previously synthesized the fluorene-linked 2'-deoxyuridine through the Suzuki coupling of 5-iodo-2'-deoxyuridine with fluorene 2-boronic acid pinacol ester. In this study, we synthesized fluorene-labeled 2'-deoxyuridine via a diacetylenyl linker and investigated its solvent-dependent photophysical properties. In addition, we incorporated it into the central position of oligodeoxynucleotide to investigate the potential as a SNP probe upon the duplex formation with fully matched and single-base mismatched targets. Detailed research results including these will be presented.

Poster Presentation : **ORGN.P-273**

Organic Chemistry

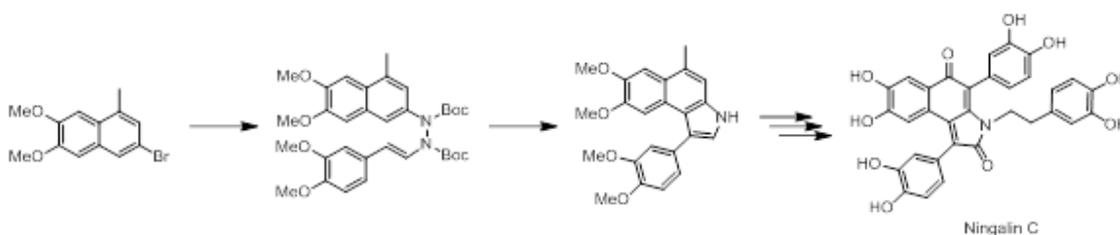
Grand Ballroom, THU 11:00~12:30

Total synthesis of natural product Ningalin C

WooHyung Kim

Hanyang University, Korea

Abstract Ningalin C is polar highly-colored alkaloid isolated in 1997 from dark purple *Didemnum* sp in Ningaloo Reef region at the northwest cape of Western Australia in the form of Dark-red amorphous powder. 1 Reaction between 5-bromo-3-methyl-2-pyrone and dimethoxy benzyne gave us synthetically useful naphthalene for natural product synthesis. With this naphthalene, we were able to synthesize key intermediates effectively. From those key intermediates, we recently had successfully synthesized ningalin D and G. 2 Recently, we have further extended the above strategy and completed the synthesis of ningalin C. The key to the success was the assembly of the indole through the successive C-N coupling reactions. Functional group transformations, oxidations and necessary substituents allowed the synthesis of the title natural product, ningalin C. Reference 1. Heonjoong Kang.; William Fenical. *J. Org. Chem.* 1997, 62, 3254. 2. Kim, J.-Y.; Kim, D.-H.; Jeon, T.-H.; Kim, W.-H.; Cho, C.-G. *Org. Lett.* 2017, 19, 4688.



Poster Presentation : **ORGN.P-274**

Organic Chemistry

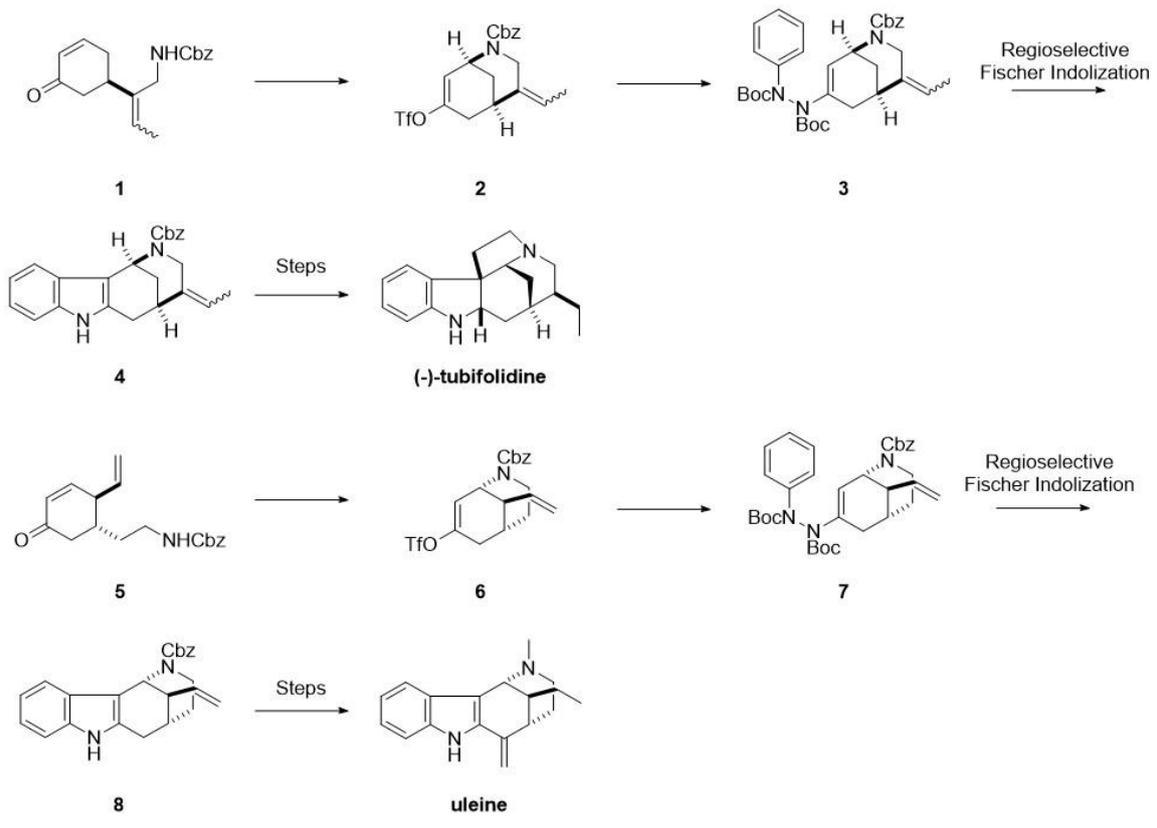
Grand Ballroom, THU 11:00~12:30

Total Syntheses of (-)-tubifolidine and Uleine via Regioselective Fischer Indole Synthesis

Jeonghwa Kim, Dong-Hyun Kim, Cheon-Gyu Cho^{*}

Department of Chemistry, Hanyang University, Korea

We have previously reported a synthesis of ene-hydrazide from enol triflate and a subsequent indolization reaction as a new entry to the regioselective Fischer indole synthesis.¹ In this process, a base-catalyzed intramolecular aza-Michael reaction, in situ trapping of the resulting enolate, and subsequent C-N coupling with phenyl hydrazide afforded the key ene-hydrazides. This new synthetic strategy has been successfully applied to the total synthesis of (+)-aspidospermidine and (-)-tabersonine.² Toward further development of our strategy, we have envisaged a new synthetic route to (-)-tubifolidine and uleine. With carbamate **1** and **5**, the carbamic anion mediated Michael addition followed by triflation will give bicyclic compound **2** and **6**. Buchwald-Hartwig type amination and regioselective Fischer indolization under Lewis acidic conditions would selectively afford desired indole **4** and **8**. Presented herein are the progress toward the syntheses of (-)-tubifolidine and uleine.



Poster Presentation : **ORGN.P-275**

Organic Chemistry

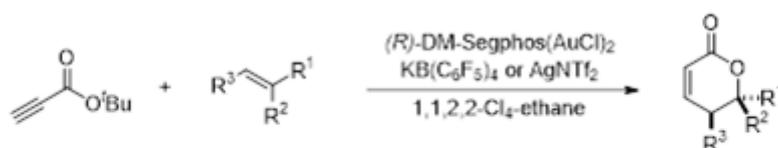
Grand Ballroom, THU 11:00~12:30

Asymmetric Synthesis of Dihydropyranones via Au(I)-Catalyzed Intermolecular [4+2] Annulation of Propiolates and Alkenes

Kim Hanbyul, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

α,β -Unsaturated δ -lactone scaffolds are found in a number of medicinal compounds displaying an array of significant biological activities. Based on the powerful alkynophilic activation of homogeneous Au(I)-catalysis, we recently demonstrated that the dihydropyranones could be assembled in a single step from the intermolecular reaction of propiolates with alkenes. However, achieving high level of enantiocontrol has remained elusive in this class of intermolecular gold(I)-catalyzed coupling. Herein, we report a highly enantioselective synthesis of α,β -unsaturated δ -lactones from [4+2] annulation of propiolates and alkenes in upto 95% ee. Notably, for the desired chiral recognition, the choice of 1,1,2,2-tetrachloroethane as solvent was found to be crucial. Furthermore, an anionic surfactant (SDS) improved the product selectivity in the divergence of the cyclopropyl gold carbene intermediate (Scheme 1).



- intermolecular asymmetric Au(I) catalysis
- control of prochiral face of olefins by (L*)Au-alkyne complex
- use of SDS in organic solvents to control selectivity

- 38 examples (63-95 %ee)
- tri-substituted and 1,2-disubstituted olefins & 1,3-dienes

Poster Presentation : **ORGN.P-276**

Organic Chemistry

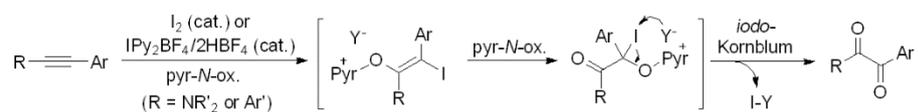
Grand Ballroom, THU 11:00~12:30

Metal-Free Iodine-Catalyzed Oxidation of Ynamides and DiarylAcetylenes into 1,2-Diketo Compounds

Tae-woong Um, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Molecular iodine has been widely used in organic synthesis, due to its easy handling and inexpensive price. Besides the stoichiometric iodofunctionalizations that incorporate iodine atom in the product, various of iodine-based catalysis have been developed, including dehydration, condensation, conjugate addition, esterification, acetalization and glycosylation. Some of these processes are suspected to be mediated by HI generated in-situ from the hydrolysis of I₂, and few reports propose a I-I regeneration for a catalyst turnover, due to the unfavorable enthalpy. Herein, we demonstrate that molecular iodine can catalyze selective oxidation of ynamide into ketoamide compounds. Ynamides as well as diaryl acetylenes are appropriate substrates for this transformation.



- chemoselectivity switch upon I^+ vs. H^+ -activation
- room temperature with low catalyst loading
- applicable to ynamides as well as non-activated alkynes

Poster Presentation : **ORGN.P-277**

Organic Chemistry

Grand Ballroom, THU 11:00~12:30

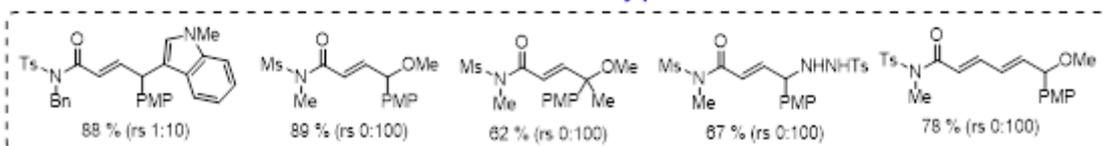
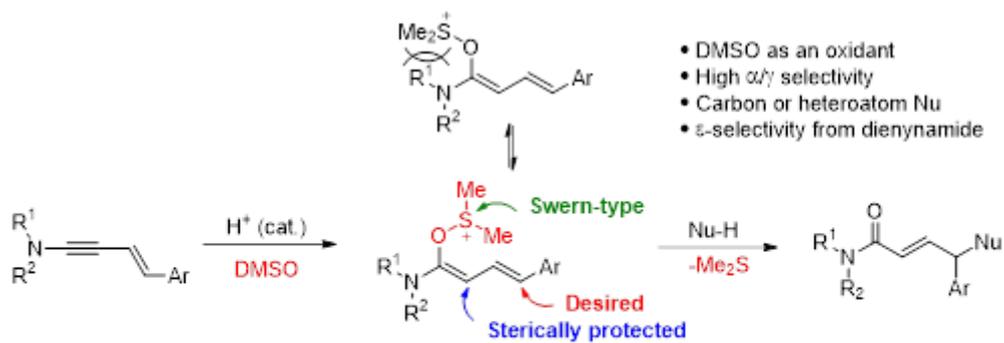
Redox Neutral Access to α^4 , α^6 -Synthons via Sulfoxide-Mediated Oxidation of (Di)enynamides

Huong Quynh Nguyen, Seunghoon Shin^{1,*}

Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Recently we have developed a robust activation of ynamides by HNTf₂ catalyst enabling oxidative coupling of diverse C-nucleophiles. This umpolung enolate discovery allows for outstanding opportunity for redox-efficient processes and enables novel disconnection approaches through non-traditional methods. We envisioned that oxidation of enynamide would provide dienolium synthon (α^4), allowing addition of nucleophilic partners at the γ -position, where the steric hindrance between amide nitrogen (N¹R²) and oxidant (OSMe₂) moiety may direct the regio-selectivity. Meanwhile, one inherent limitation in the gold- or Brønsted acid-catalyzed oxidation of alkynes is the necessity to use pyridine-derived N-oxides as terminal oxidant which liberates pyridine that undermines atom-economy and potentially inhibits the acid-catalyzed cycle. Employing dimethyl sulfoxide (DMSO) as terminal oxidant led to an efficient γ -selective couplings without intervention of side pathways. In addition to carbon nucleophiles, 1°, 2°-alcohols and tosyl hydrazide could be employed as nucleophiles. Using dienynamides as substrates, ϵ -addition (α^6) could be realized with excellent selectivity.



Poster Presentation : **MEDI.P-278**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Novel Aminoquinazolinyloindolines and Their Enzyme Inhibitory and Anticancer Activities

Juseung Kim, Juri Suh, Sunwoo Lim, Jongseung Kim¹, Kyung Ho Yoo^{2,*}

Chemical Kinomics Research Center, Korea Institute of Science and Technology / Department of Chemistry, Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

²*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

In recent years, AXL kinase has emerged as a key facilitator of immune escape and drug-resistance by eliminating intercellular antibodies, regulating the release and secretion of cytokines. AXL has been implicated as a cancer driver and correlated with poor survival in numerous aggressive tumors including TNBC, AML, NSCLC, pancreatic cancer, and ovarian cancer. The ACK1 tyrosine kinase is aberrantly activated, amplified, or mutated in many types of human cancers, including prostate, breast, pancreatic, ovarian, and lung cancers. Therefore, AXL and ACK1 have been proposed as the attractive targets for cancer therapeutics and a number of small molecule inhibitors have been developed. The purpose of this study is to develop the potent compounds as dual kinase inhibitors against AXL and ACK1. Based on the structural features of TP-0903 and TAE-684 as AXL and ACK1 inhibitors, a novel series of aminoquinazolinyloindoline derivatives were designed and synthesized. Their *in vitro* enzyme inhibitory and antiproliferative activities were tested. Among them, several compounds showed good inhibitory activities against AXL and ACK1. Many compounds showed potent antiproliferative activities against MV4-11 and A549 cell lines with GI₅₀ values of sub-micromolar range. In our series, compound **1m** possessing 4-methylpiperazinylphenylamino moiety exhibited good inhibitory activities (IC₅₀ = 0.887 and 6.16 μM, respectively) against AXL and ACK1, together with potent antiproliferative activities (GI₅₀ = 0.0237, 0.762, and 0.752 μM for MV4-11, A549, and HeLa, respectively).

Poster Presentation : **MEDI.P-279**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Novel function of DNMT inhibitors to suppress prions

Jiaojie Li^{*}, Chunyan Ren¹

Dept of Chemistry, Gwangju Institute of Science and Technology, China

¹*Structural and Chemical Biology, Icahn School of Medicine at Mount Sinai, United States*

The conversion of the normal cellular prion protein (PrPC) to the misfolded pathogenic scrapie prion protein (PrPSc) is the biochemical hallmark of prion replication. Various chemical compounds that inhibit this conformational conversion have been identified. Here, we present the anti-prion activity of SGI-1027 and its meta/meta analog (M/M), known as potent inhibitors of DNA methyltransferases (DNMTs). These compounds effectively decreased the level of PrPSc in cultured cells with permanent prion infection, irrespective of PrPC suppression at the transcriptional and translational levels, via DNMT inhibition. Furthermore, SGI-1027 prevented effective prion infection of the cells. In a PrP aggregation assay, both SGI-1027 and M/M blocked the formation of misfolded PrP aggregates, implying that binding of these compounds hinder the PrP conversion process. A series of binding and docking analyses demonstrated that both SGI-1027 and M/M directly interacted with the C-terminal globular domain of PrPC, but only SGI-1027 bound to a specific region of PrPC with high affinity, which correlates with its potent anti-prion efficacy. Therefore, SGI-1027 and related compounds represent potential anti-prion agents that operate through direct interaction with PrPC.

Poster Presentation : **MEDI.P-280**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Development of 3D Bio-Printing Model for In vitro & In vivo Test

Sang Hyeob Lee, Il Yoon^{1,*}

Department of Nanoscience, Nano Drug Delivery Lab, Korea

¹PDT Laboratory, Inje University, Korea

Recently, 3D bioprinting has much attention for development of model systems for in vitro as well as in vivo in cancer therapy. In this poster, we will show current progress of 3d bioprinting using biocompatible materials, such as hydrogel and polymers. 3D scaffolds were fabricated by various parameters, such as speed, nozzle size, pressure and so on.

Poster Presentation : **MEDI.P-281**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

**[Withdrawal] Synthesis of radioprotective agents through modification
of the anticancer compound.**

Minjeong Kim, Jung Hwan Choi, Inhee Choi, Kaapjoo Park*

Medicinal Chemistry, Institut Pasteur Korea, Korea

- Withdrawal -

Poster Presentation : **MEDI.P-282**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Tetrahydroazepines as β -arrestin biased ligands of 5-HT7R

Jieon Lee, Hyunah Choo^{1*}, Youngjae Kim²

Center for Neuromedicine, Korea Institute of Science and Technology, Korea

¹Korea Institute of Science and Technology, Korea

²Department of Chemistry, Yonsei University, Korea

5-HT7 receptor (5-HT7R) is the most recently described member of the 5-HT receptor family. Autoradiographic and immunohistochemistry studies in human, guinea pig, and rat CNS showed that 5-HT7R is distributed in discrete areas with high to moderate concentration in limbic areas, such as the thalamus, hypothalamus, hippocampus, and amygdala, in the raphe and cortical regions. On the basis of its distribution in the CNS, 5-HT7R was proposed to be involved in important roles such as circadian rhythm, sleep, learning and memory well as several diseases such as migraine, sleep disturbance, and depression. 5-HT7R belongs to the family of G protein coupled receptors (GPCRs) and is shown to be positively coupled to adenylate cyclase through activation of Gs-proteins. Particularly, not only G proteins but also non-G protein effectors such as β -arrestin are involved in GPCR signaling. The so-called “functionally selective” or “biased” ligands are believed to stimulate either G protein signaling pathway or β -arrestin signaling pathway independently. The development of potent and selective biased ligands of 5-HT7R would be of great help in understanding the relationship between pharmacological effects and G protein/ β -arrestin signaling pathways of 5-HT7R. Herein, we designed and synthesized tetrahydroazepine derivatives 1 and 2 with arylpyrazolo moiety or arylisoxazolo moiety. Through several biological evaluations such as binding affinity, selectivity profile, and functions in G protein and β -arrestin signaling pathways, tetrahydroazepine derivative 1g was discovered as the β -arrestin biased ligand of 5-HT7R. In addition, we evaluated the effect of 1g on electroencephalogram (EEG) sleep architecture to investigate a correlation between β -arrestin biased activity of 1g and NREM/REM sleep pattern in mice.

Poster Presentation : **MEDI.P-283**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

A novel orally active inverse agonist of estrogen-related receptor gamma (ERR γ), DN200434, increase the susceptibility of radioiodine therapy against anaplastic thyroid cancer through upregulation of sodium iodide symporter (NIS) function

Jina Kim, Jungwook Chin^{1,*}, Sung Jin Cho^{1,*}

Department of Chemistry, Daegu Gyeongbuk Medical Innovation Foundation, Korea

¹New Drug Development Center, Daegu Gyeongbuk Medical Innovation Foundation, Korea

New strategies to restore sodium iodide symporter (NIS) expression and function in anaplastic thyroid cancers (ATCs) that are refractory to radioiodine therapy are urgently required. Based on the structural motifs of GSK5182, we have successfully demonstrated the synthesis of compound libraries that are more selective against ERR γ inverse agonists with improved absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles. Moreover, we have broadened the therapeutic scope of these compounds based on our findings that GSK5182 facilitates the responsiveness to radioiodine therapy by modulating NIS function in ATC cells via ERR γ and MAP kinase signaling pathway. Herein, we have validated the most promising ERR γ inverse agonist, DN200434, from our previous studies for its ability to enhance NIS protein function, which is a key protein for radioiodine therapy, and improve susceptibility to the therapy in in vitro/vivo ATC models.

Poster Presentation : **MEDI.P-284**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Studies on SHP2 inhibitors for Cancer Treatment

Bohee Kim, Seungjin Jo¹, Jeong-Hun Sohn, Byumseok Koh¹, Inji Shin^{1,*}

Department of Chemistry, Chungnam National University, Korea

¹Therapeutics & Biotechnology Division, KRICT, Korea

SHP2, non-receptor protein tyrosine phosphatase encoded by PTPN11 gene, plays an important role in the control of cell growth, oncogenic transformation and differentiation. Activating mutations of SHP2 have been reported as a cause of Noonan syndrome and several cancers, such as leukemia or breast cancer. The discovery of SHP2 inhibitor can be a therapeutic candidate for the treatment of cancers and SHP2 associated diseases. Studies on a small molecule targeting protein tyrosine phosphatases (PTPs) have been challenged due to polarity of the catalytic site. Therefore, discovery of an allosteric inhibitor can be a good alternative to an active site inhibitor. Herein, we present our research on SHP2 inhibitors. Through high-throughput screening (HTS), we identified a 'hit', and further study is currently in progress.

Poster Presentation : **MEDI.P-285**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Extracellular-matrix proteins delivery system for tissue regeneration

Huong Thanh Nguyen, Kilyong Lee¹, Minyoung Kim, Agustina Setiawati², Sungwoo Jeong, Nahee Kim, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

¹Disease Biophysics Group, Wyss Institute for Biologically Inspired Engineering, United States

²Department of Life Science, Sogang University, Korea

Wound healing is an essential physiological process in which tissue repair and regeneration occur after injury. The lack of several factors for wound healing such as growth factors and extra-cellular matrix (ECM) has been observed in hard-to-heal wounds. Drugs developed from growth factors failed to provide expected outcome; therefore, ECM proteins approach is emerging as a promising alteration. Human neonatal dermal fibroblasts were used for in vitro experiments. Either pure liposomes, fibronectin or fibronectin coated on liposomes were delivered to the cells. WST-1 cell proliferation assay and fluorescence live-cell imaging were performed to evaluate cell growth and migration in each group. Mouse model of ulcerative colitis induced by acetic acid was used for in vivo experiments. HE staining of the colon tissues and measurement of inflammatory cytokines level were performed in our study. We found a significantly faster growth in the cells in which liposomes coated by fibronectin (FN) were delivered. Moreover, in in-vitro scratch assay, this group has remarkably shorter recovery time compared to the control group. In vivo data confirmed that the mice treated with FN-coated liposomes had less tissue damage than other groups after 10 days of treatment. Our results revealed that fibronectin, when coated to liposomes prior to delivery to cells, can have significantly higher effect in wound healing than when delivered with no carrier. This enables the ability to develop a wound healing material using our SUV-based ECM delivery system. The underlying mechanism of the wound healing process facilitated by this system remains to be revealed in further studies.



Extracellular matrix proteins-liposome delivery system for tissue regeneration

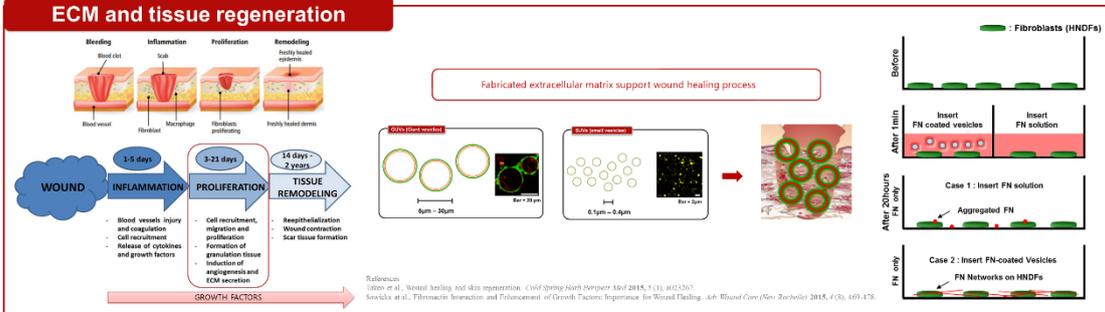
Huong Thanh Nguyen¹, Kilyong Lee^{1,3}, Minyoung Kim¹, Agustina Setiawati^{1,2}, Sungwoo Jeong¹, Nahee Kim¹, Kwanwoo Shin^{1,4}

¹Department of Chemistry and Institute of Biological Interfaces, Sogang University, Republic of Korea

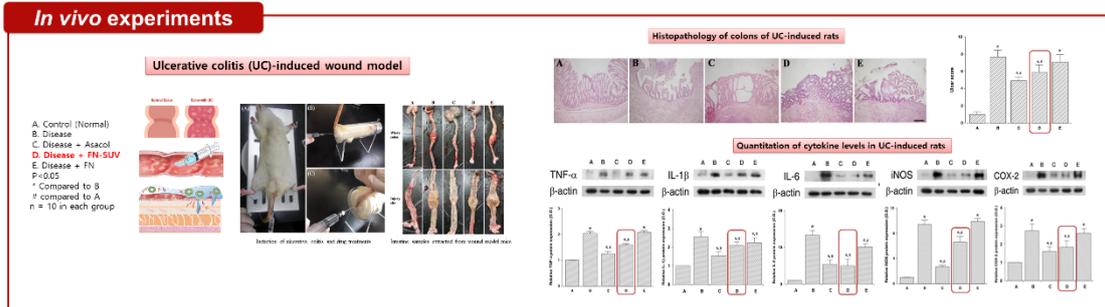
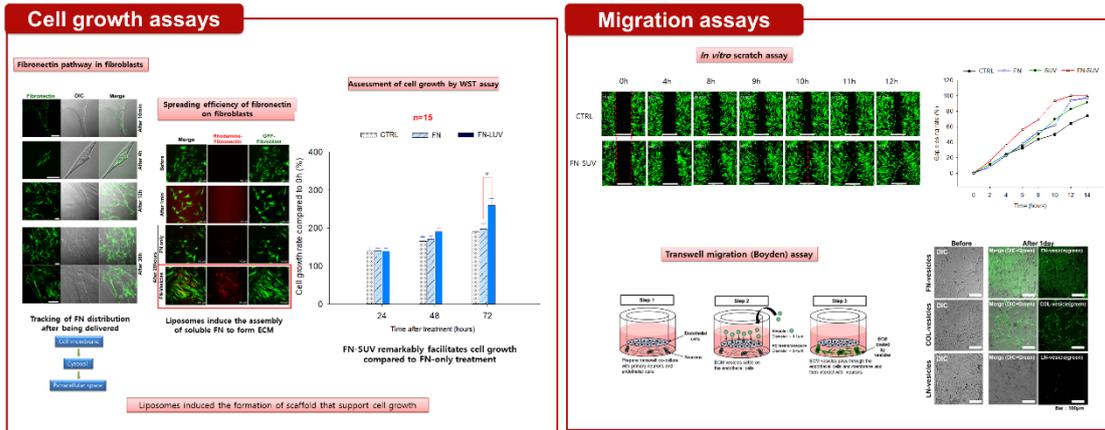
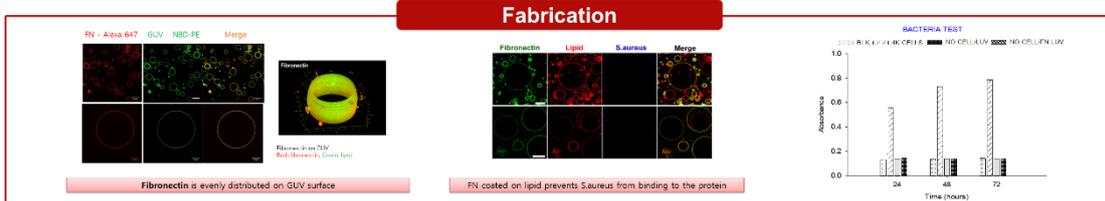
²Department of Life Science, Sogang University, Republic of Korea

³Disease Biophysics Group, Wyss Institute for Biologically Inspired Engineering, John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA

Introduction



Experimental Details and Results



Poster Presentation : **MEDI.P-286**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Studies on the discovery of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

**HyoJin Kim, HyeonJeong Jeong¹, Yun Kyung Kim², Ae Nim Pae², Cheol-Hong Cheon^{*},
Sang Min Lim^{2,*}**

Department of Chemistry, Korea University, Korea

¹*Korea University, Korea*

²*Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is one of the most common neurodegenerative diseases that must be studied because it becomes a serious problem in an aging society. Although AD has been extensively studied, there are only drugs that alleviate some of the symptoms of Alzheimer's disease, and there are no disease-modifying drugs. Tau is a microtubule associated protein (MAP) that binds to and stabilizes microtubules. However, hyperphosphorylation of tau induces the separation from the microtubules, and the separated tau self-assembles forming tau oligomers and aggregates that result in induction of neuronal loss and eventually neurodegenerative diseases such as AD. Therefore, we develop tau aggregation inhibitors to find drug candidates for the treatment of AD. To discover new hit compounds that can inhibit tau aggregation, we performed a high-throughput screening based on Bi-FC assay with in-house compound libraries. By modifying hit compounds, we have found compounds that are more potent and less toxic than Methylene blue: a well-known in vitro tau aggregation inhibitor. Currently, a variety of derivatives have been synthesized through a structure-activity relationship study to find compounds that are more potent than the hit compounds. We will continue to work to further optimize potency as well as physicochemical properties to develop clinical candidates.

Poster Presentation : **MEDI.P-287**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

(-)-Epigallocatechin (EGC) shows methylglyoxal (MGO)-trapping activity and thereby inhibitory activity against advanced glycation end product (AGE) formation

Eunryeol Shin, Youhoon Chong*

Department of Biotechnology, Konkuk University, Korea

Maillard reaction is a multistep non-enzymatic process which includes the reaction of glucose with free amino groups of proteins leading to the formation of highly reactive advanced glycation end products (AGEs). AGE modification of proteins and thereby damages to cells and tissues have been confirmed to contribute to the pathophysiology of aging and long-term complications of various age-related diseases. The major reactive carbonyl compound that forms AGEs is methylglyoxal (MGO), and trapping and inactivating MGO have been recognized as the most viable approach to anti-AGEs therapy. In this study, we have shown strong MGO-scavenging activity of (-)-epigallocatechin (EGC). EGC was equipotent to previously identified MGO-scavengers such as (-)-epigallocatechin gallate (EGCG) and quercetin. Also, EGC inhibited protein glycation caused by MGO.

Poster Presentation : **MEDI.P-288**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Paeonol Derivatives and their Cholinesterase Inhibitory Activity toward Development of Alzheimer's Drug Candidates

Cheolmin Jeon, Yujung Kang^{*}, Haneul Lee, Jeong Ho Park^{1,*}

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Alzheimer's disease (AD) is the most common neurodegenerative disease among the cause of dementia which can appear in the elderly people aged 65 or old. The cause of Alzheimer's disease is not yet known exactly. Alzheimer's drugs based on the cholinergic theory currently marketed for the treatment of AD patient. However, they have some side effects. We have been researching to find out new candidate compounds as cholinesterase inhibitors. In this study, a series of paeonol compounds were synthesized and their *in vitro* cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated. The structure-activity relationship (SAR) study depended on the Claig plot was carried out ; plotting the sigma constants of the Hammett equation (σ) versus hydrophobicity (π). The IC₅₀ value of compound 5 (+ σ , + π) is $0.26 \pm 0.06 \mu\text{M}$ and it is comparable to that of galantamine (IC₅₀ = $12.74 \pm 0.86 \mu\text{M}$ against BuChE).

Poster Presentation : **MEDI.P-289**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Anti-oxidative compounds and tyrosinase inhibitory compounds from *Fallopia japonica*

Zhou Xinxin^{*}, Gyusun Jeong¹, Heesu Kwon¹, Bong Ho Lee^{2,*}, Byong Wook Choi^{1,*}

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In our continuing search for biologically active compounds from oriental medicinal plants, *Fallopia japonica* was examined. Here, we documented the progress on the purification, biological activities and structural determination of the purified compounds. From the 100% methanol extract of *Fallopia japonica*, solvent partition were prepared by using *n*-hexane (FJH), chloroform (FJC), butanol (FJB) and water (FJW). Among them, the extracts in FJB possessed strong anti-oxidative and anti-tyrosinase activities. The extracts in FJB of *Fallopia japonica* showed 89.9% DPPH radical scavenging activity, and 67.2% tyrosinase inhibitory activity at 100 ppm. Using a series of ODS (octadecylsilyl) open column chromatography, four compounds, 13-FJB-282, 13-FJB-283, 13-FJB-4832 and 13-FJB-52, were purified. The chemical structures of 13-FJB-282, 13-FJB-283, 13-FJB-4832 and 13-FJB-52 were determined by ¹H and ¹³C NMR and comparison of HPLC chromatogram with reference compounds. 13-FJB-282 was turned out to be Piceid. Our results suggest that four compounds extracted from *Fallopia japonica* showed strong anti-oxidative and anti-tyrosinase activities.

Poster Presentation : **MEDI.P-290**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

EGCG derivatives reduce the expression of both urokinase plasminogen activator and plasminogen activator inhibitor-1 to show anti-metastatic activity

Sunhye Shin, Youhoon Chong*, Kim Yoonjeong

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Urokinase plasminogen activator (uPA) and its inhibitor plasminogen activator inhibitor-1 (PAI-1) are established independent biomarkers for high metastasis risk in breast cancer. In this study, we investigated the regulatory activity of EGCG and its derivatives on uPA and PAI-1 expression and thereby their anti-metastatic potential. EGCG showed only marginal effects on the uPA system and on the metastatic behavior of breast cancer cells (MDA-MB-231). However, the EGCG derivatives showed potent inhibition of PAI-1 and uPA expression. The Ras-extracellular-signal-regulated kinase (ERK), p38 mitogen-activated protein kinase (MAPK), and phosphatidylinositol-3-kinase (PI3K)/Akt/NF- κ B pathways, which regulate uPA and PAI-1 expression, were also affected by EGCG derivatives. In line with these findings, substantial reduction in metastatic behavior of MDA-MB-231 cells, such as adhesion, invasion, and migration, was observed in the presence of EGCG derivatives. Taken together, we have shown that the EGCG derivatives could suppress the metastatic behavior of MDA-MB-231 cells through regulation of uPA and PAI-1.

Poster Presentation : **MEDI.P-291**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Discovery of novel anti-tubercular agent for the treatment of MDR/XDR TB

Jung Hwan Choi, Youkyeong Song, Aram Lee, Guanghai Jin, Inhee Choi, Kaapjoo Park*

Medicinal Chemistry, Institut Pasteur Korea, Korea

Given the high attrition rate during clinical development and emergence of resistance, the discovery of additional antitubercular clinical candidates is clearly needed. There is still unmet medical need so discovering potent agents capable of reducing the treatment time of MDR/XDR TB patients with a success rate comparable to that of current therapies for drug-susceptible tuberculosis is in high demand as of today. We have identified a novel scaffold, TTCA, which showed potent inhibitory activities against extracellular and intracellular bacteria. Around 360 derivatives of TTCA have been synthesized so far. Interestingly, TTCA compounds have better potency against intracellular bacteria. Also, TTCA compounds were active against tested clinical MDR strains with MIC less than 1 μ M. In vitro ADME and physicochemical properties profiling suggested that TTCA series have drug-like properties. In addition, TTCA series showed pharmacokinetic and safety profiles of druggable characteristics. Herein, we report on finding of a novel TTCA scaffold that could effectively inhibit TB. Especially, TTCA compounds have the potentials to be developed as treatment for latent TB. Together, our data indicates that TTCA compounds are promising novel clinical candidates for the treatment of MDR/XDR TB.

Poster Presentation : **MEDI.P-292**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Discovery of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

Haeun Lee, Ae Nim Pae^{1,*}, Sang Min Lim¹

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¹*Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is one of the most common neurodegenerative diseases and becomes a severe problem in an aging society. Tau protein plays an important role in AD pathology. Tau is a microtubule-associated protein and, helps to stabilize neuronal microtubule. But hyperphosphorylation of tau leads to disengage it from the microtubule, which results in self-assembly of tau forming paired helical filaments (PHFs) and neurofibrillary tangles (NFTs). Finally, these PHFs and NFTs induce neuronal damage like AD. Although tauopathy has been extensively studied as a key hypothesis in AD there are no clinical drugs to give the noticeable improvement. Therefore, we study to find Tau-directed therapeutic drug candidates for the treatment of AD, especially, tau aggregation inhibitors. To discover new lead compounds that can inhibit tau aggregation, we performed a high-throughput screening based on Bi-FC assay with in-house and commercial compound libraries. Subsequently, we found hit compounds that are more potent and less toxic than the Methylene blue: a well-known in vitro tau aggregation inhibitor. Currently, a variety of derivatives were synthesized through a structure-activity relationship study to find compounds that are more potent and possess novel scaffolds than the hit compounds. We will continue to work to further optimize potency as well as physicochemical properties to develop clinical candidates.

Poster Presentation : **MEDI.P-293**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Biological Evaluation of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

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Alzheimer's disease (AD) is a neurodegenerative disease and the most common cause for dementia. With the advent of an aging society, the importance of Alzheimer's disease is increasing. However, there is currently no treatment options that can completely cure AD. Neurofibrillary tangles (NFTs) are one of the main hallmarks of AD and primarily composed of tau protein. In the AD patient's brain, tau protein, which stabilizes microtubules is hyperphosphorylated and then self-aggregates to form NFTs. NFTs induce neuronal damage resulting in diseases like AD. We envisaged that inhibition of the formation of NFTs would be beneficial for the treatment of AD, and therefore we are developing tau aggregation inhibitors. Through screening based on tau-BiFC (bimolecular fluorescence complementation) assay with in-house and commercially available compound libraries, we found promising hit compounds. They showed excellent tau aggregation inhibitory activity, but some of their drug-like properties need to be improved to be AD drug candidates. Therefore, we are optimizing hit compounds to further increase potency and drug-like properties, including BBB (brain-blood barrier) penetration.

Poster Presentation : **MEDI.P-294**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Asymmetric squaraines bearing N-substituted Fischer's base moieties as anticancer photosensitizers: Synthesis, characterization and biological evaluation

Hyoung-jin Choi, JuEun Kim, Hyejin Jeong, So-young Ma¹, Jong dae Lee*, Bee Kim

Department of Chemistry, Chosun University, Korea

¹*Center for Photovoltaic Materials, Korea University, Korea*

Condensation of squaric acid with N-substituted Fischer base moieties containing electron-donating substituents gave only the semisquaraines. However, with salts possessing electronegative and electron-withdrawing groups, the squaraine dyes were isolated in good yields. The semisquaraines formed undergo condensation with other N-substituted Fischer base yielding the asymmetrical squaraine dyes. These results demonstrate the role of electronic factors and provide valuable information for the design of efficient squaraine-based sensitizers that can have potential applications in photodynamic therapy.

Poster Presentation : **MEDI.P-295**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Spiropyran bearing N-substituted Fischer's base moieties as anticancer photosensitizers: Synthesis, characterization and biological evaluation

Se-young Park, Bee Kim, JuEun Kim, Hyejin Jeong, So-young Ma¹, Jong dae Lee*

Department of Chemistry, Chosun University, Korea

¹Center for Photovoltaic Materials, Korea University, Korea

Reversibly controlled generation of singlet oxygen from photosensitizing spiropyran systems has the benefits of selective cell killing and controllable effect time, but is a challenging option for photodynamic therapies. We found that Fischer's base-containing various spiropyran dyes have photoswitching properties for both fluorescence and singlet oxygen generation in aqueous solutions and cells, and demonstrated that spiropyran dye featuring induced enhanced photosensitization and emission could be potentially applied in photodynamic therapy studies on tumor cells.

Poster Presentation : **MEDI.P-296**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Epigallocatechin-3-Gallate (EGCG) Conjugated with Phenylalanine Shows Stimulation of Hepatic Autophagy and Lipid Clearance

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¹*Department of Biotechnology, Konkuk University, Korea*

(-)-Epigallocatechin gallate (EGCG) is known as an autophagy-enhancing and thereby lipid-lowering agent, and optimization of its activity warrants its therapeutic potential in the treatment of hepatic diseases as well as metabolic disorders. In this study, we investigated the autophagy-enhancing activity of 14 EGCG derivatives and, among those, E10 with a phenylalanine attached to the 4"-O-position of the EGCG scaffold showed the most promising effects in stimulating autophagy in Huh7 cells: 1) stimulation of autophagy was demonstrated by an increased amount of LC3B-II as well as the activation of a key enzyme for the initial autophagy process (AMP-activated protein kinase, AMPK) in the presence of E10; 2) E10-stimulated autophagic flux was confirmed by an increase in LC3B-II upon co-treatment with chloroquine (CQ), reduction of p62/SQSTM1, and increase in the formation of autophagic compartments visualized by both CYTO-ID staining and tandem RFP-GFP-LC3 fluorescence. Finally, the autophagy-inducing activity of E10 culminated in a reduction of hepatic lipid accumulation caused by fatty acids. In all of the assay settings performed in this study, E10 was consistently 1.3 to 3.5-fold more potent than EGCG. Taken together, we demonstrated a significant increase in autophagy stimulating activity of EGCG through structural modifications, which opens the door to an extensive structure-activity relationship study of the EGCG scaffold for the discovery of more potent autophagy enhancers.

Poster Presentation : **MEDI.P-297**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

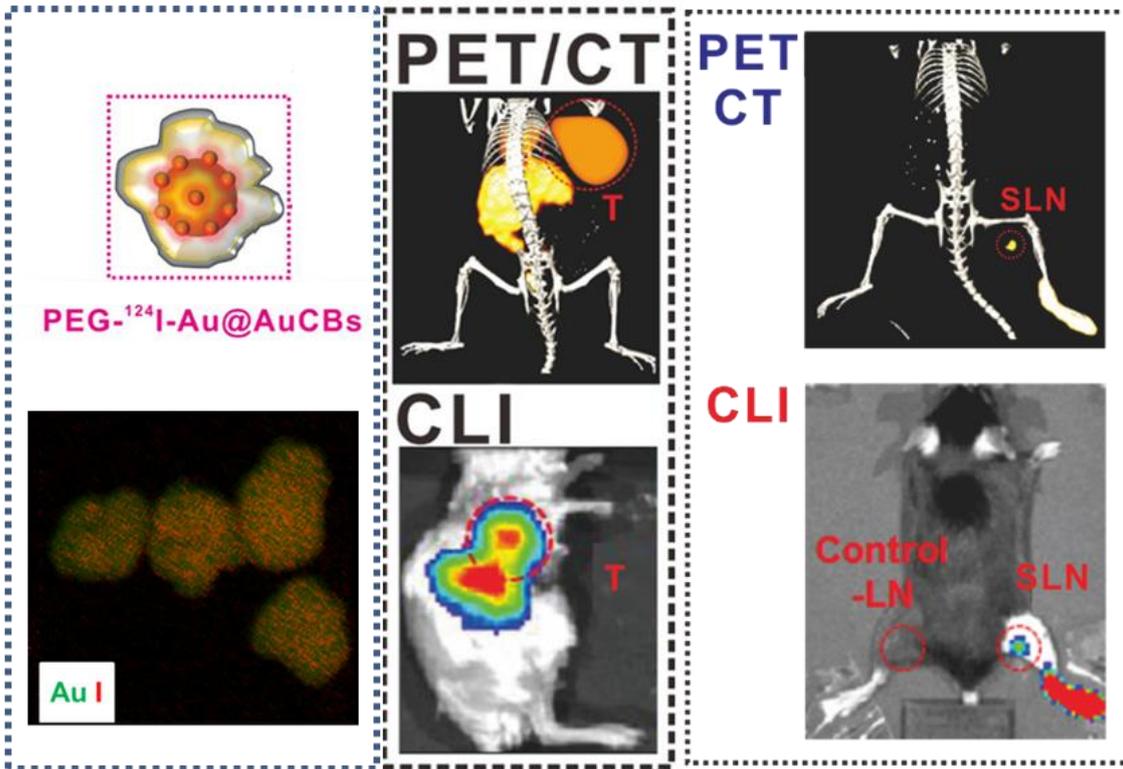
PEGylated crushed gold shell-radiolabeled core nanoballs for in vivo bio imaging application with dual positron emission tomography and cerenkov luminescent imaging

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Radioactive isotope labeled gold nanomaterials have potential biomedical imaging applications. Here, we report the synthesis and characterization of PEGylated crushed gold shell-radioactive iodide-124 labeled gold core nanoballs (PEG-124I-Au@AuCBs) for in vivo biomedical imaging application through combined positron emission tomography and cerenkov luminescent imaging (PET/CLI). PEG-124I-Au@AuCBs showed high stability and sensitivity in various pH solutions, serum, and in vivo conditions and were not toxic to tested cells. Combined PET/CLI clearly revealed disease lesions at 1 to 24 h after injection of particles, consistent with the biodistribution results. Taken together, the data provided strong evidence for the application of PEG-124I-Au@AuCBs as promising imaging agents in nuclear medicine imaging of various biological systems, particularly in diagnostics of various disease.



- T : Tumor SLN : Sentinel lymph nodes

Poster Presentation : **MEDI.P-298**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Loreclezole as a new class of potent insect growth regulators with mosquitocidal activity

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The mosquito is about 3500 species exist on the earth and they mediate diseases such as malaria, dengue fever, Zika virus, Japanese encephalitis, epidemic, chikungunya and this like. Recently, Insect growth regulators (IGRs) could become an effective target to control mosquitoes by having selectivity to insects and relatively low toxicity. Juvenile hormone (JH)-based IGRs including JH agonists (JHAs) and antagonists (JHANs) fatally affect the physiological regulations in insects and are effective for control the target insects. In this study, we introduce the Loreclezole as a novel JH-based insect growth regulator by the two-hybrid yeast β -galactosidase assay method in a yeast cell from chemical library. To investigate the relationship of loreclezole analogues between chemical structure and JHA activity, we prepared Loreclezole derivatives and obtained their activities in vivo test. To evaluate the mosquito larvicidal activities of loreclezole and its analogues with high JHA or JHAN activities, the mortality of 3rd instar larvae of *Aedes albopictus* treated with these compounds was determined. Among these compounds, K8363A and K9001C showed the highest mosquitocidal activity.

Poster Presentation : **MEDI.P-299**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and biological evaluation of pyrimidine derivatives as selective 5-HT_{2C} ligands

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Serotonin (5-HT) is one of the major neurotransmitters that is primarily located in the central nerve system (CNS) and plays an important role in the regulation of a variety of physiological functions such as intestinal movements, mood, cognition, appetite and psychiatric diseases. 5-HT receptors, e.g., 5-HT_{1A}, 5-HT_{2A}, and 5-HT_{2C} subtypes, may also play a role in cognitive and motivational disabilities in psychoses and mood disorders. For example, several antipsychotic and antidepressant drugs have been suggested to ameliorate negative symptoms and mood disturbances, partly through actions on 5-HT_{1A} and 5-HT_{2A} receptors. Clozapine, a prototype of atypical antipsychotic drugs, which is most effective in treating negative symptoms of schizophrenia, may act as an inverse agonist on 5-HT_{2C} receptors. It has been studied that neurotransmitters such as dopamine (DA) and 5HT are directly/indirectly associated with psychiatric disorders. More recently, interest has emerged in the therapeutic potential of compounds with agonistic activities at 5-HT_{2C} receptors to address unmet medical needs across the symptom domains of schizophrenia. Although several compounds have been identified as 5HT_{2C} agonists, new compounds with high selectivity against other 5-HT subtypes are still requested for clinical development. Herein, we describe synthesis and evaluation of pyrimidine derivatives as selective 5-HT_{2C} ligands. We have identified several compounds showing high binding affinity toward 5-HT_{2C} receptors. We also found that those pyrimidine analogues displayed excellent agonistic activity in cell-based functional assay. Further evaluation of these compounds regarding selectivity and stability will be addressed in this presentation.

Poster Presentation : **MEDI.P-300**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Screening of Gram-positive specific antibacterial agents

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¹Division of Chemical Engineering, Yeungnam University, Korea

Antimicrobial resistance (AMR) pathogens suggested that the deaths attributable to AMR will exceed 10 million per annum by year 2050. There is unmet need to eradicate AMR bacteria is developing specific, high-efficiency, and non-toxic antibiotics. In this study, new chemicals were synthesized by a novel method. Synthesized chemicals were further evaluated antibacterial activity against *S. aureus*, *E. coli*, and *P. aeruginosa*. Of the total 63 chemicals, four chemicals (KS-16, -17, -19, -22) showed good antibacterial activity against Gram-positive bacteria in terms of zone of inhibition (>10 mm). Furthermore, the measurement of MIC values showed that four chemicals were comparable to commercial antibiotic, streptomycin against *S. aureus*. Therefore, four compounds could be used as a platform for making new antibiotics against anti-*S. aureus*. In the future, it is necessary to identify antibiotic mechanisms of these compounds.

Poster Presentation : **MEDI.P-301**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of EGCG-amide and its specific cytotoxicity against highly metastatic breast cancer (MDA-MB-231) cells

Taegum Lee, Youhoon Chong*, Sunhye Shin

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(-)-Epigallocatechin gallate (EGCG), a major green tea flavonoid, is well known for its cytotoxic activity against various cancer cell lines. In this study, a new EGCG derivative with an amide linkage at the C3 position was synthesized by using oxidation followed by reductive amination strategy of the globally protected epigallocatechin. The newly synthesized EGCG-amide was investigated for its anticancer activity against a panel of cancer cell lines to show strong cytotoxicity against the highly metastatic breast cancer cells (MDA-MB-231). Given the importance of metastasis in the cancer treatment, the mechanism for specific cytotoxicity of the EGCG-amide against the MDA-MB-231 cell lines is of particular interest. Synthesis, anticancer activity, and identification of the target proteins of EGCG-amide will be presented.

Poster Presentation : **MEDI.P-302**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Development of novel Quinoline Derivatives for a Fluorescent Imaging Probe with Binding Selectivity to tau

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¹Korea Institute of Science and Technology, Korea

²Chemoinformatics Research Center, Korea Institute of Science and Technology, Korea

Alzheimer's disease (AD) is one of the chronic neurodegenerative disease and the most common cause of dementia. Post-mortem studies of AD brains have revealed two pathological hallmarks of the disease. The first one is extracellular amyloid beta (A β) plaques which affect the interaction between neuronal process at synapse. And the second is intracellular neurofibrillary tangles (NFTs) formed by tau protein, also disrupt on synaptic function. Tau proteins stabilize microtubules in neurons. By abnormal mutation or hyperphosphorylation, tau proteins separated from microtubules. Separated tau proteins form insoluble PHF-tau (paired helical filament) and NFTs by self-aggregation. In the recent research, the density of A β plaques doesn't correlate well with the progress of neurodegeneration or cognitive impairment in AD. In contrast, the density and neocortical spread degree of NFTs correlate well with progressive neuronal degeneration and cognitive decline in AD patients. Thus NFTs are the desirable biomarker for AD and the binding selectivity to tau over A β is needed to develop a probe for diagnosis the AD. It is reported that some quinoline moieties are specifically targeting tau aggregates. In this research, we designed and synthesized the quinoline derivatives that is 2,6-disubstituted by electron withdrawing groups or electron donating groups based on the donor- π -acceptor architecture for developing the fluorescent imaging probe that has selectivity to tau over A β . The result of in vitro studies about selectivity and fluorescence intensity will be presented in detail.

Poster Presentation : **MEDI.P-303**

Medicinal Chemistry

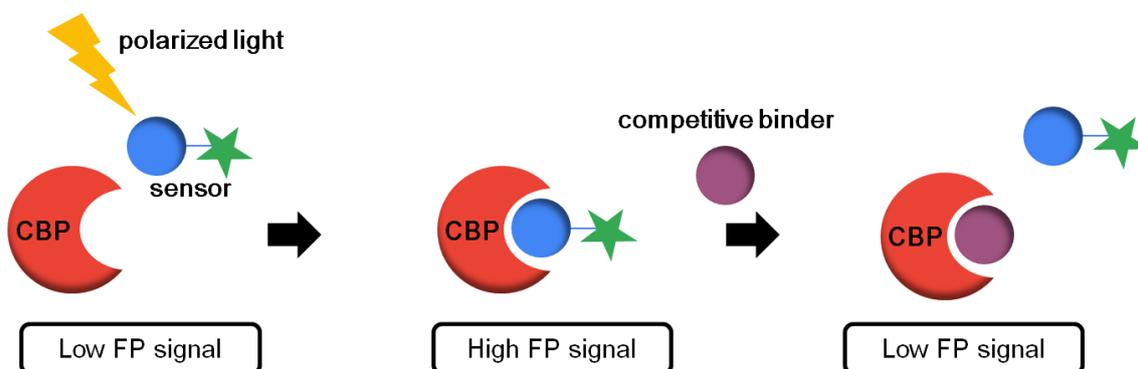
Grand Ballroom, THU 11:00~12:30

Development of a High-Throughput Fluorescence Polarization Assay for Discovery of a Inhibitor for CBP bromodomain

Jinhyo Hwang, Hak Joong Kim*

Department of Chemistry, Korea University, Korea

The single bromodomain of a transcriptional regulator called cAMP response element binding protein (CBP) has attracted much interest as a target for cancer and immune modulation. For instance, some inhibitors recently reported by Genentech have showed marked anti-proliferative effects in hematologic cancers primarily by suppressing MYC expression. Here, we describe development of a new fluorescence polarization (FP) assay that can be optimized for a high-throughput screening to identify novel CBP bromodomain inhibitors. Specifically, a number of fluorescent tracers were newly designed by covalent conjugation of a known CBP bromodomain inhibitor with a fluorescein dye. This assay was validated against a panel of competitive ligands based on the excellent Z' score. We believe that this new FP assay platform could be a simple and reliable alternative to conventional assays for evaluating CBP bromodomain inhibitors such as TR-FRET- or AlphaScreen-based systems.



Poster Presentation : **MEDI.P-304**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

CRISPRgo: Ressurrection of Non-sense mutated gene expression by ABE.

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CRISPR-Cas9 systems are broadly applicable in genome engineering fields. In early stage of CRISPR-Cas9 system, the aim of using CRISPR-Cas9 focused on DNA cleavage and gene Knock-out. However, now we are facing new application of using CRISPR-Cas9 system, such as Cytidine Base-editor(BE) and Adenine Base-editor(ABE). BE and ABE induces much less insertion or deletion than does Cas9. That mean we can achive intending genetic modification without the genomic damage that may inducing cell death or unexpected genetic mutations. Moreover, ABE is a adenine base editro which is substitutes A to G. Using the ABE, we can change the STOP codon (TAA, TAG, TGA) into the other amino acid (Trp, Gln and Arg). Therefore, ABE is able to restore the gene expressions which are stoped by non-sense mutation. In this study, We demonstrated the capblity of ABE, restoring non-sense mutation, in EGFP expression prevented by whole stop codons. We compared three kinds of ABE (Cas9 ABE 7.10, xCas9 3.7-ABE3 7.10 and ABE-max) efficiency in EGFP-stop cell line by FACS and NGS results. Futhermore non-sense mutation is critical in genetic diseas, therefore we did restore the gene expression in patient's fibroblast, such as XPC, GAA, and ENPP1 genetic diseas. Finally, ABE is an effiective system for restoring stoped gene expression without inducing the genetic damage by double strand DNA cleavages.

Poster Presentation : **MEDI.P-305**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Pharmaceutical composition for the treatment of dry eye syndrome from Terminalia chebula

**Bong Geun Song, Pilju Choi¹, Joonseong Hur², Seon-Jun Choi, Young-Tae Park², Jun
Hyuk Choi³, Sang Il Jeon, Jungyeob Ham^{2,*}**

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³*Chung-Ang University, Korea*

Dry eye syndrome (DES) is an eye disease known as keratoconjunctivitis sicca, which causes defects in the eye and tear film due to various causes. Common symptoms include irritation, foreign body sensation, light sensitivity, and itching. Anti-inflammatory drugs such as corticosteroids and cyclosporine are also used as treatments for dry eye syndrome. However, there were risk of side effects such as glaucoma and cataract in long-term use. To solve the problems, we studied for the prevention and treatment of dry eye syndrome using natural products. In this presentation, we found that Terminalia chebula extracts or fractions play a crucial role in preventing or treating dry eye syndrome, and will show the therapeutic effect of dry eye syndrome through Terminalia chebula extract and fractions in In-vivo.

Poster Presentation : **MEDI.P-306**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

3,5-Disubstituted indole derivatives as Pim kinase inhibitors

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Department of Chemistry, Keimyung University, Korea

Pim kinases (Pim-1, Pim-2, and Pim-3) are involved in many cellular processes such as survival, growth, cell cycle, proliferation and cell's metabolism. Pim kinases are frequently overexpressed in multiple cancer including solid tumors, leukemia and lymphoma. Pim kinases are an attractive therapeutic target in the development of anti-cancer agents. A novel series of 3,5-disubstituted indole derivatives were synthesized as Pim kinases inhibitors. Synthesized compounds showed potent inhibitory activities against Pim kinases. The most potent compound exhibited IC₅₀s of 0.003 μ M for Pim-1 and 0.007 μ M for Pim-3.

Poster Presentation : **MEDI.P-307**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Design and Solid-Phase Parallel Synthesis of 2,4,5-Trisubstituted Thiazole Derivatives as a Potential Sphingosylphosphorylcholine (SPC) Receptor Inhibitors

Hyejin Kwon, Sun Hwa Jung, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

In this study, we prepared library of 2,4,5-trisubstituted thiazole derivatives via solid-phase synthesis by introducing various electrophile substituents such as acyl halide, alkyl halide to the 2,4-diamino(thiazole-5-yl)substituted-phenylmethanone resin. We are expecting that synthesized 2,4,5-trisubstituted thiazole derivatives will show biological activity against SPC receptor because 2,4-disubstituted-5 aminocarbonyl-1,3-thiazole derivatives is already known as a good therapeutic agent toward SPC. SPC plays a multifunctional role such as cell growth, differentiation, calcium signaling, tissue remodeling. Prominent skin disorders, such as psoriasis and atopic dermatitis, have diminished epidermal ceramide levels, reflecting altered SPC metabolism. In previous studies, the sulfone traceless linker was introduced to the Merrifield resin for the synthesis of 2,4,5-trisubstituted thiazole derivatives. However, this methodology only can give diversity to 2,4-diamino(thiazole-5-yl)substituted-phenylmethanone resin using nucleophile substituents. To improve the diversity of compounds, we have decided to introduce new carbamimidothioate linker to the Merrifield resin thus linker will act as a nucleophile and allow to introduce various electrophile substituents. As a result, an improved molecular diversity of the 2,4,5-trisubstituted thiazole library can serve more effectively in the development of a potential SPC receptor inhibitors.

Poster Presentation : **MEDI.P-308**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of 2-Amino-5-Carboxamide Thiazole derivatives via Dehydrative Cyclization of Thiourea Intermediate Resin on Solid Phase

Ye Ji Kim, Min Jeong Cha¹, Young Dae Gong*

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¹*Dongguk University, Korea*

In this study, we synthesized 2-amino-5-carboxamide thiazole derivatives on solid phase. The synthesis of library starts from the reductive amination of the 4-formyl-3-methoxy phenoxy resin to prevent isomer formation. The dehydrative cyclization of thiourea intermediate resin, which is the key step of the synthetic process, was successfully conducted with using α -bromoketone in the presence of the dimethylformamide to afford 2-amino-5-carboxylate thiazole resin. The resulting resin undergoes amide coupling with various amines. Finally, the 2-amino-5-carboxamide thiazole resin was cleaved from the polymer support under trifluoroacetic acid in dichloromethane. Additionally, physicochemical properties of constructed 2-amino-5-carboxamide thiazole derivatives were conducted. According to the study results, the library molecules show reasonable oral bioavailability drug properties as determined by the Lipinski's Rule.

Poster Presentation : **MEDI.P-309**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Design and Synthesis of Novel Drug-Like 4-(1,3,4-oxadiazol-2-yl)piperazine-2,5-dione Library via Microwave Assisted Combinatorial Chemistry

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We have been interested in compounds containing 2,5-piperazinedione and 1,3,4-oxadiazole due to its wide range of biological activities. In this reason, we aimed to construct 4-(1,3,4-oxadiazol-2-yl)piperazine-2,5-dione libraries. The key step in this synthetic methodology is the formation of 2,5-piperazinedione by cyclization of methyl 2-(2-(amino)acetamido)acetate. Even though several synthesis routes of 2,5-piperazinedione core skeleton derived from a reaction between *N*- α -chloroacetyl amino acid methyl ester and amines on solution-phase have been published, those reaction conditions generate the desired compound in low yields and require long time. Accordingly, we developed efficient route for the preparation of 2,5-piperazinedione derivatives via microwave assisted combinatorial chemistry. Microwave irradiation can reduce reaction time rapidly and give higher yields and purities compared to conventional thermal heating. So, we obtained 2,5-piperazinedione in a effective way successfully. Next, 2,5-piperazinedione intermediates are reacted with phenyl chloroformate and hydrazides in order. Finally, we can synthesize 1,3,4-oxadiazole derivatives by dehydrative cyclization. We expect that this affording library will show good therapeutic efficacy.

Poster Presentation : **MEDI.P-310**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Discovery constipation drug using aminoalkylbenzothiazepine derivative

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Chronic idiopathic constipation is highly prevalent among adults. Bile acids (BAs) and the enterohepatic BA circulation modulate colonic secretion and motility that affect transit. BAs in the colon have a dual action as osmotic and stimulant agents. Newer agents, such as CJ-compounds, an inhibitor of the ileal BA transporter, have the potential to improve significantly the management of chronic constipation, with minimal adverse effects. Utilized the strategy adopted in the design of Elobixibat and GSK compound, we prepared several analogs based on core part scaffold of Elobixibat and GSK compound. Primary focus was to increase potency in vitro. The SAR studies described in this project focused side chain, aromatic substitution. Compound A has non-absorbable properties and it optimized to get efficacy. Finally, we can found more potent CJ compounds than Elobixibat. CJ compounds, an IBAT inhibitor, modulates the enterohepatic BA circulation, and increases BA synthesis enhancing the delivery of BAs to the colon to increase colonic motility, and secretion and fecal excretion of BAs. CJ compounds has significant effects on the manifestations of chronic constipation with minimal and tolerable adverse effects. Compound A exhibited potent and selective IBAT inhibition and effectively improved treatment constipation. These results warrant further investigation of compound A as a promising candidate for patient who needs treatment of constipation.

Poster Presentation : **MEDI.P-311**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Predictive QSAR model for potential eye irritation of organic chemicals

Kang Min Lee, Meiyu Zhang, Sung Kwang Lee*

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Evaluating the eye Irritation potential of a chemical is a necessary procedure in the risk assessment. We are exposed to various eye irritants in cosmetics, ocular pharmaceuticals, household products, manufacturing industries and etc. *Draize test* was used a standard protocol to evaluate the eye irritant potential of a chemical. However, It has several limitations such as highly cost and time-consuming and cruelty of using rabbit's tissue. Therefore, the QSAR model for evaluating eye irritation can be a solution to these problems.

The data used in the development of QSAR model is **MMAS**(Modified Maximum Average Score) data according to OECD Guideline 405, and vapor pressure data, collected from QSAR Toolbox 4.2, PhysProp database, eChemPortal database and several literatures. All data consist of 60% of their training set for the model learning by selecting the most diverse structure set, and 40% of external sets.

In this study, a QSAR prediction model was constructed by using multiple linear regression(MLR) and support vector machine(SVM) methods and all models were verified using y-scrambling and external validation. Through these studies, we have analyzed the substructures(structure alerts) that can cause eye irritation. This predictive model is expected to be useful for development of cosmetic materials and drug screening research.

※ Acknowledgement

This research was supported by a grant (**18182MFDS466**) from the **Ministry of Food and Drug Safety** in 2018.

Poster Presentation : **MEDI.P-312**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

**[Withdrawal] QSAR modeling of the acute contact toxicity to
honeybees**

Young eun Song, Meiyu Zhang, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

- Withdrawal -

Poster Presentation : **MEDI.P-313**

Medicinal Chemistry

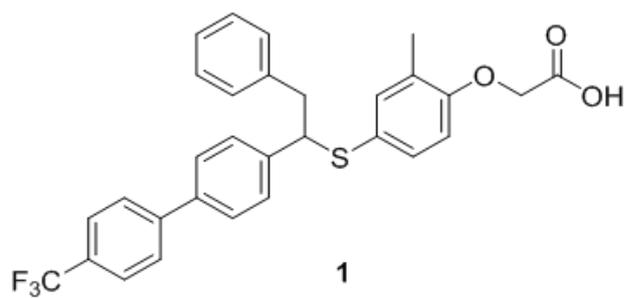
Grand Ballroom, THU 11:00~12:30

Development of “Y”-Shaped Biaryl Peroxisome Proliferator-Activated Delta Agonist

Dong-Su Kim, Su-Jeong Lee, Jungwook Chin*, Sung Jin Cho*

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

Peroxisome proliferator-activated receptors which comprise three subtypes (PPAR alpha, delta and gamma) have recently received significant attention due to their function as transcription factors that regulate gene expression patterns of biological processes. Among these subtypes, PPAR delta is related to various metabolic diseases. In this regard, diverse strategies for development of PPAR delta modulators have been widely studied. Recently, GlaxoSmithKline discovered highly potent and selective PPAR delta agonists such as GW501516 and GW610742. Based on these model compounds, several types of PPAR delta agonists have been devised. To this extent, GW501516 modified “Y”-shaped PPAR delta specific agonists were reported by Kang group. Evans group also reported new type of “Y”-shaped PPAR delta agonists. Based on these works, we designed and synthesized various “Y”-shaped biaryl PPAR delta agonists. Structure-activity relationship (SAR) analysis was performed to find title compound **1** that the most active agonist with an EC₅₀ of 2.6 nM. Activity of enantiospecific *R* and *S* isomers of compound **1** was confirmed that *R* isomer (EC₅₀ = 0.7 nM) shows much more potent activity than *S* isomer (EC₅₀ = 6.1 nM). Molecular docking studies between the PPAR ligand binding domain and enantiospecific *R* and *S* isomers of compound **1** were conducted. In vitro absorption, distribution, metabolism, excretion, and toxicity (ADMET) and in vivo PK profiles show that compound **1** involves reasonable drug-like properties and good bioavailability. Our overall results clearly demonstrate that this orally available PPAR delta agonist **1** is a viable drug candidate for the treatment of PPAR delta-related diseases.



- readily accessible synthetic route
- high selectivity for PPAR δ
- high potency (PPAR δ : EC₅₀ = 2.6 nM)
- suitable ADMET profile
- appropriate PK profile for p.o. dosing

Poster Presentation : **MEDI.P-314**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Anti-Atherosclerotic and Lipid-Lowering Effects of the Mixture of Crataegus pinnatifida Fruit and Lycopus lucidus

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Development of atherosclerosis is caused by a high concentration of LDL-cholesterol in the blood. This study was to investigate the possibility of the lipid-lowering and anti-atherosclerotic effects of the mixed extracts of *Crataegus pinnatifida* Fruit and *Lycopus lucidus* (MCL) in human umbilical vein endothelial cells (HUVECs) and Poloxamer-407 (P-407) mouse model, and to explore its underlying mechanism. For confirmation of reproducibility of MCL, we conducted a fingerprint using high performance liquid chromatography (HPLC)-based compositional analysis, with four main compounds including protocatechuic acid, quercetin dehydrate, chlorogenic acid, and cirsilineol respectively. In HUVECs, MCL inhibited tumor necrosis factor (TNF)- α -induced THP-1 monocytes adhesion to the HUVECs as well as up-regulation of vascular cell adhesion molecule-1 (VCAM-1) and intercellular adhesion molecule-1 (ICAM-1). In mouse models, serum lipid levels (total cholesterol, TC; triglycerides, TG; and low-density lipoprotein cholesterol, LDL-C) were increased significantly in the P-407-induced group as compared to the normal group. Interestingly, MCL administration caused a significant reduction in serum TC (p

Poster Presentation : **MEDI.P-315**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

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Alzheimer's diseases (AD) is a chronic neurodegenerative disease that is most common case of dementia. The hallmarks of Alzheimer's diseases are the senile plaque which is composed of Amyloid beta ($A\beta$) peptide and neurofibrillary tangles (NFTs) consisted of mainly hyperphosphorylated tau protein in the brain. Recent studies have suggested that inhibition of lipid phosphatase known as SH2 domain-containing inositol 5'-phosphatase 2 (SHIP2) rescued tau hyperphosphorylation and improved memory impairments. Furthermore, interaction between SHIP2 and Fc γ RIIb is critical in $A\beta_{1-42}$ induced tau pathology. The binding of $A\beta_{1-42}$ to Fc γ RIIb induces ITIM phosphorylation and SHIP2 is recruited to interact with Fc γ RIIb. SHIP2 increases Ptdins(3,4)P₂ levels by dephosphorylation of 5-phosphate group from Ptdins(3,4,5)P₃ resulting in Gsk3 β activation followed tau hyperphosphorylation. Therefore, Inhibition of SHIP2 protein can be a potent therapeutic strategy for $A\beta_{1-42}$ induced tau hyperphosphorylation pathology in AD. In order to discovery SHIP2 hit compounds, the phosphatase assay with malachite green carried out our in house and commercial compound libraries. The high-throughput screening produced, several hit compounds and we synthesized new derivatives based on the scaffolds of hit compounds. Consequently, we could find out some compounds with improved physicochemical properties. The optimization of novel SHIP2 inhibitor is now in progress and these compounds will be help to understand physicochemical functions of SHIP2 and pathological pathways of AD.

Poster Presentation : **MEDI.P-316**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Design and Synthesis of a Novel Class of pirazolo-triazine compounds as SIRT6 Activators

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¹new medical development, Chungbuk Natioanl University, Korea

For the development of a new SIRT6 Activator, we synthesized N-methyl-N-phenylpyrazolo[1,5-a][1,3,5]triazin-4-amine (1). 5-Amino-1H-pyrazole-1-carboxamide (2) was synthesized and built to Pyrazolo[1,5-a][1,3,5]triazin-4(3H)-one (3) . Following N-methyl-N-phenylpyrazolo[1,5-a][1,3,5]triazin-4-amine (4) was obtained and reacted in iodination. Various functional group was reacted with this pirazolo-triazine in the presence of Suzuki catalysis to give N-methyl-N-phenylpyrazolo[1,5-a][1,3,5]triazin-4-amine structure (6), which was converted into the corresponding several compounds (7). Structure-activity relationships of (6) and (7) were investigated.

Poster Presentation : **MEDI.P-317**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Enhancing dual gene delivery efficiency using tannic acid to form AAV complex

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Chemical and Biomolecular Engineering, Yonsei University, Korea

Adeno associated virus (AAV) is a promising method for gene therapy. However, the biggest drawback of AAV is that it can only carry certain sizes of DNA. To overcome this situation, many scientists cut DNA in several suitable sizes to fit in AAV. Nevertheless, it shows low number of gene expression because all the DNA need to be injected to the target cell to be functional. The tannic acid works as a bond to hold different viruses together, which forms AAV complex. The efficiency of dual gene delivery increases as AAV complex gains entry into a cell. By using this novel AAV complex method, it will effectively deliver genes to the target cell.

Poster Presentation : **MEDI.P-318**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Ginsenoside Rb2 suppresses multiple mechanisms of glutamate mediated neurotoxicity in HT22 cells

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The neuroprotective effects of ginsenosides were evaluated using glutamate induced neurotoxicity model. Among the ginsenosides, Rb2 shows protective effect against glutamate mediated neuronal cell death using HT22 cells. To investigate mode of action of Rb2 in neuroprotective effect, we analyzed cellular Ca²⁺ and reactive oxygen species (ROS) level, which is trigger to apoptosis through activation of MAPK and AIF translocation. Image analysis using DCFDH and Flu3 shows Rb2 block Ca²⁺ influx and accumulation of cellular ROS. Western blot analysis shows that Rb2 inhibits MAPK activation and AIF translocation by initiating glutamate induced oxidative stress. Further animal study using the Mongolian gerbil of ischemic brain injury mouse model also shows Rb2 strongly inhibits brain ischemic injury. We currently undertake structural elaboration to improve Rb2 delivery to brain.

Poster Presentation : **MEDI.P-319**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Optimization of Vinyl Sulfone Derivatives as Potent Nrf2 Activator for Parkinson's Disease Therapy

Ji Won Choi, Siwon Kim, Jong-Hyun Park, Hyeon Jeong Kim, Su Jeong Shin, Ki Duk Park*

Convergence Research Center for DTC of Dementia, Korea Institute of Science and Technology, Korea

We previously developed a novel series of vinyl sulfones as Nrf2 activators with a therapeutic potential for Parkinson's disease (PD). However, the previously developed lead compound (**1**) exhibited undesirable drug-like properties such as solubility, metabolic stability, CYP inhibition and hERG safety. Here, we have optimized a class of vinyl sulfones introducing pyridine and morpholine moieties to improve drug-like properties. Among the synthesized compounds, **17e** is the most promising drug candidate with excellent drug-like properties such as good solubility, high human microsomal/plasma stability, low CYP inhibition and excellent hERG safety. In addition, **17e** showed superior effect on Nrf2 activation in the cell based assay compared to compound **1** (**17e**; EC₅₀:346 nM vs **1**; EC₅₀:530 nM). **17e** was further confirmed to induce expression of the Nrf2-dependent anti-oxidant enzymes NQO1, GCLC, GCLM, and HO-1, at both mRNA and protein levels. In the MPTP-induced mouse model of PD, **17e** significantly attenuated the loss of tyrosine hydroxylase (TH)-immunopositive dopaminergic neurons, suppressed microglial activation, and alleviated the PD-associated motor dysfunction. In conclusion, we present **17e** as a novel Nrf2 activator with excellent drug-like properties and potential therapeutic candidate for PD.

Poster Presentation : **MEDI.P-320**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Neuroprotective Effects of Nrf2 Activator via Inhibition of Protein-protein Interaction in a Mouse Model of Parkinson's Disease

Siwon Kim, Jong-Hyun Park, Ji Won Choi, Su Jeong Shin, Hyeon Jeong Kim, Hyeon Ji Kim, Ae Nim Pae*, Ki Duk Park*

Convergence Research Center for DTC of Dementia, Korea Institute of Science and Technology, Korea

Parkinson's disease (PD) is a neurodegenerative disorder characterized by abnormal movement, including slowed movements, shuffling gait, lack of balance, and tremor. Recently, oxidative stress was shown to play a critical role in dopaminergic neuronal cell death in PD. The nuclear factor E2-related factor 2 (Nrf2)-Kelch-like ECH-associated protein 1 (Keap1) signaling pathway provides the main defense system against oxidative stress by inducing the expression of antioxidant enzyme genes. Direct interference in the Keap1-Nrf2 protein-protein interaction (PPI) has emerged as an effective strategy for Nrf2 activation. Therefore, we searched for small-molecule PPI inhibitors that can act as Nrf2 activators by using a virtual screening approach and identified a potent Nrf2 activator, KKPA4026. KKPA4026 was confirmed to induce the expression of the Nrf2-dependent antioxidant enzymes heme oxygenase-1, glutamate-cysteine ligase catalytic subunit, glutamate-cysteine ligase regulatory subunit, and NAD(P)H:quinone oxidoreductase 1 in BV-2 cells. In an MPTP-induced mouse model of PD, KKPA4026 effectively attenuated PD-associated behavioral deficits and protected dopaminergic neurons.

Poster Presentation : **MEDI.P-321**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Evaluation of Novel Functionalized Amino Acid Derivatives for Treatment of Cryptococcal Meningitis

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Cryptococcus and *Candida* are the representative opportunistic fungus that causes fungal inflammation in a group of people whose immune system is impaired by aging or medical issues such as organ transplantation, chemotherapy, and AIDS. Especially, *Cryptococcus neoformans*, a type of the *Cryptococcus*, is easily found in soil, bird excrement. Its basidiospores are inhaled into the lungs through the respiratory system, and cryptococcal pathogens in the body cause inflammation in the lung and eventually leads to meningitis when penetrating the central nervous system (CNS) through the blood-brain barrier (BBB). In this study, we have synthesized a series of functionalized amino acid (FAA) derivatives for the development of antifungal agent against *C. neoformans* and evaluated their potency using in vitro antifungal susceptibility test (Minimal inhibitory concentration (MIC)). In a previous study, we derived the potent leading compound KDS1090 through MIC testing for representative fungal pathogens. (MIC: *C. neoformans* = 4 g/mL, *C. albicans* = 16 g/mL, *C. glabrata* = 16 g/mL). Herein, we optimized lead compound for both the antifungal efficacy and drug-like properties. Among the optimized compounds, KDS5098 showed the highest antifungal efficacies (MIC: *C. neoformans* = 2 g/mL, *C. albicans* = 4 g/mL). Furthermore, KDS5098 exhibited excellent ADME/Tox profiles (microsomal stability (human): 90%, (mouse) 78% remaining after 30 min; CYP inhibition (1A2, 2C9, 2C19, 2D6): IC₅₀ > 10 μM, (3A4; 56% inhibition at 10 μM); single dose toxicity (mice): LD₅₀ > 1,000 mg/kg; PK: F=40%).

Poster Presentation : **MEDI.P-322**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

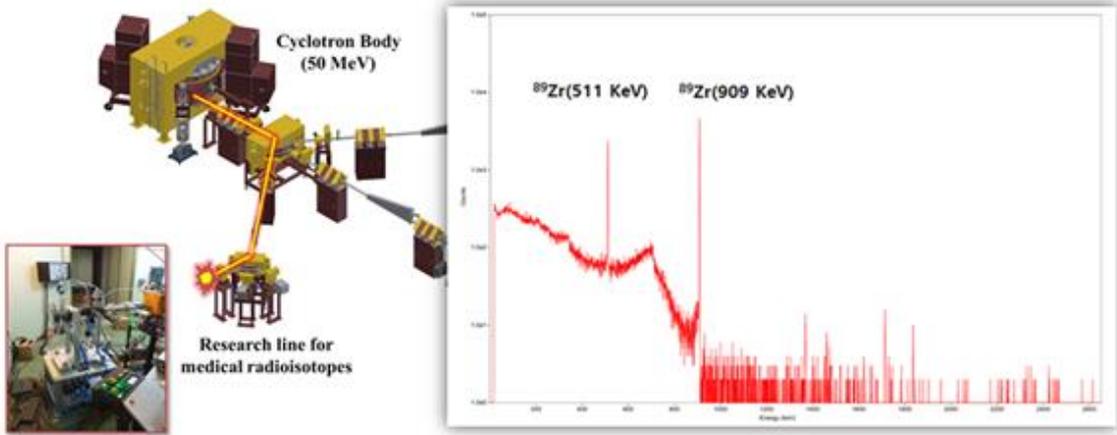
Production Study of Medical Radioisotope Zirconium (^{89}Zr) by the Deuteron Beam of 50 MeV Cyclotron

**Sangjin Han, Hyun Park, Choong Mo Kang¹, Ji Ae Park, Yong Jin Lee, Kyo-Chul Lee,
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A radioactive zirconium (Zr-89 , half-life 3.27 days), one of zirconium isotopes, is positron-emitted radioisotope, and it has recently been used for immuno-PET in nuclear medicine. In particular Zr-89 has been developed as radioisotope-labeled antibody conjugates with bifunctional chelate agents, and shows good tumor PET imaging in human studies. Therefore, it needs novel production study of Zr-89 as the daily increased demand of many researchers and medical doctors. Zr-89 has been generally produced from the nuclear reaction of Y-89(p,n)Zr-89 by proton beams of commercially baby cyclotron. However, the nuclear reaction has not showed high radioactivity of Zr-89 due to the limit of baby cyclotron. To overcome the low yield of Zr-89 by previously production skills, we studied for Zr-89 production by the nuclear reaction of Y-89(d,2n)Zr-89 using the deuteron beam of high energy, with new target station. The new Y-89 target and its station here was exclusively developed for deuteron beam, and it was dissolvable by a mixed acid solution. The mixture solution went through a specific short column of hydroxamate resin, and then Zr-89 of high radiochemical purity could be obtained as the chemical form of Zr-89 oxalate. To remove excess oxalate, it added more purification step using QMA. We were successful to finally produce 12-15 mCi/h of high purified Zr-89 . The result showed 3-4 times higher than the radiochemical yield of proton beam at Zr-89 production. It wasn't also observed any radiochemical impurities except both 511 and 909 KeV of inherent gamma energies of Zr-89 . The purified Zr-89 chloride here could be labeled with DFO-Bz-NCS of bifunctional chelate agents. We could be successfully produced as Zr-89 of high purity and yield by the deuteron beam of 50 MeV cyclotron.



Poster Presentation : **MEDI.P-323**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and biological effects of hydrogen sulfide donor peptide hybrids.

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Hydrogen sulfide (H₂S) has been known as a critical signaling molecule that regulates many physiological and/or pathological processes. With the multiple biological actions of H₂S, there is growing interest in developing various H₂S-releasing compounds for precise delivery of the gas to target tissues. Recently, the connection between drug and H₂S-delivery components has led to a considerable variety of H₂S donors with potential therapeutic effects against diseases. In our group, hydrogen sulfide (H₂S)-releasing dithiolethione (ADT) functionalized with biologically active peptides are being investigated for their integrated anti-inflammatory and antioxidant potential. Herein, we report the synthesis of a series of H₂S-releasing compound peptide hybrids and their initial biological effects.

Poster Presentation : **MEDI.P-324**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Naked-eye sensitive detection of tuberculosis specific antigen based on copper-gold enhancement immunoassay

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Department of Chemistry, Chung-Ang University, Korea

Conventional diagnosis procedures for identifying biomarker such as microbiological test, immunological test, biochemical processes required long time duration, labour-intensive instruments, exorbitant costs and caused false results. Silver nanoshell enhancement on the gold nanoparticles (AuNPs) surface is usually performed in immunoassay platform to intensify the colorimetric signal for the detection of biomarkers but lack of selectivity and sensitivity limit its application as a biodetection label. Herein, a straightforward and highly specific dot-blot immunoassay was successfully developed to detect Mycobacterium tuberculosis secretory antigen, CFP-10, based on copper nanoshell formation on the AuNPs surface. The reduction capacity of sodium L-ascorbate to the Cu-PEI complex can form the copper nanoshell on the AuNPs surface, results in the double amplification of the optical signals than that of conventional silver nanoshell. For biomarker diagnostics, this strategy was applied to detect CFP-10 tuberculosis antigen, and the magnified signals can be strongly detectable with naked-eye or a smartphone camera with the detection limit as low as 8 pg/mL. A simple copper enhancing bioassay can identify the CFP-10 antigen in clinical urine sample with high sensitivity, specificity, low cost as well as minimization of complicated procedures. This facile and sensitive bioassay exhibits great application potential for highly reliable point-of-care detection of other biomarkers in biomedical field or life science

Poster Presentation : **MEDI.P-325**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Mini-Review of biological applications of various free base and metalocorrole

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Department of Pharmaceutical Science, Jungwon University, Korea

Recently corrole compounds, which have very similar core structure with porphyrin, have been attracted many interests with respect to synthetic strategies and biological applications. Although photophysical properties of corroles are similar porphyrin molecules, it has been known that biological characteristics exhibit more improved applicability for molecular imaging, detection and degradation of tumors, nucleic acid regulators, catalytic degradation of reactive oxygen/nitrogen species (ROS/RNS), anti-microorganism and generation of singlet oxygen as photosensitizers. Herein, we reviewed various free base- and metallo-corroles and their biological applications.

Poster Presentation : **MEDI.P-326**

Medicinal Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of A2B corroles for the application of photodynamic therapy

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Many researches are interested in developing tumor-specific destruction method. As an alternative therapeutic skill, photodynamic therapy (PDT) attracts great interests due to its high temporal and spacial selectivity to tumor cells. PDT is based on the photosensitizers which can generate singlet oxygen by energy transfer from triplet excited state sensitizers to molecular oxygen in ground state. Herein, we designed two types of free base A2B corroles and phosphorus corroles as photosensitizers, synthesized, and characterized the photophysical properties via measuring of UV-vis absorbance, and emission spectra, etc. For the next step, we are planning to synthesize various halogenated metallocorroles and investigating phosphorescence properties and application for tumor removal potential in cellular level.

Poster Presentation : **MAT.P-327**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

The novel strategies for developing CO₂ absorbent based on MgO

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An endeavor for reducing the concentration of CO₂ in atmosphere induces the development of carbon capture utilization and storage (CCUS) technologies. The concept of this technology is to capture, separate CO₂ from an anthropogenic point source and use it to the chemical reagents or store in underground. In order to realize CCUS technology, the development of CO₂ absorbent is an urgent issue. The concept of triple stage CO₂ absorption proposed by Park et al. make MgO a prominent material to be used in the intermediate temperature range (200-500 °C). We used the different phase of promoters such as solid and molten state alkali metal salts with additives and compared CO₂ absorption performance. Based on the above experimental results, we propose CO₂ absorption and desorption mechanisms of MgO promoted by alkali salts. In order to enhance the stability of the absorbents, we introduce ZrO₂ dispersant to the solid alkali carbonate-promoted MgO absorbent. Finally, we suggest novel strategies for improving MgO based CO₂ absorbent. Detailed results will be presented in a poster session.

Poster Presentation : **MAT.P-328**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Spray Coating of Brown Algae-Derived Fucoidan for Antibacterial Applications

**Soojeong Cho, Woo Kyung Cho^{*}, Joon Sig Choi¹, Sung Min Kang², Sangwon Ko³,
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Bacteria can adhere to various surfaces and rapidly proliferate, forming biofilm. Biofilm can serve as a reservoir of spreading the bacterial cells and can be crucial problems for public health. To prevent bacterial contamination on surfaces, antibacterial materials and their coating methods have been studied. Herein, we synthesized an antibacterial material by introducing catechol group into brown algae (*Fucus vesiculosus*)-derived fucoidan via amide coupling. Spray coating method, which can be applied to large surface area, was devised through the crosslinking between ferric ion and catechol-conjugated fucoidan. The catechol-conjugated fucoidan (FD-C) was applied to stainless steel and titanium dioxide and the fucoidan-coated substrates were characterized by using ellipsometer, contact angle goniometer, Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy, and atomic force microscopy. We demonstrated that the FD-C coated substrates have antibacterial property, compared to bare substrates, using *E. coli*. We also applied the spray coating of fucoidan to straps of train and confirmed the antibacterial effect of the spray coating. We think this approach can be utilized for antibacterial coatings for equipment in public transportation to prevent infectious harmful substances from spreading.

FD-C Spray Coating

Fucoidan catechol (FD-C)

Poster Presentation : **MAT.P-329**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Fabrication of Noble Metal coated $\text{Fe}_3\text{O}_4@\text{TiO}_2$ with Enhanced Photocatalyst Activity

Kyeong-Mi Song, Keum-Chul Seo, Jin-Seung Jung*

Department of Chemistry, Gangneung-Wonju National University, Korea

With a growing demand for clean and comfortable environment, purification technologies with high efficiency and low cost to reduce the pollutant contents of wastewater are urgently needed. TiO_2 is considered to be one of the suitable material for photocatalysts due to its nontoxicity, biological inertness, chemical stability and low-cost. In addition magnetic Fe_3O_4 particles have been introduced to functionalize core-shell particles due to their unique separable feature that makes it possible to realize convenient recycling of novel metals. In this study, a facile and efficient approach for fabricating Ag-coated $\text{Fe}_3\text{O}_4@\text{TiO}_2$ particles with a good core-shell structure is demonstrated. The Ag-coated $\text{Fe}_3\text{O}_4@\text{TiO}_2$ photocatalyst exhibited high photocatalytic activity in the degradation of Rhodamine B (Rh.B) under solar light. Finally, the photodynamic process of Ag-coated $\text{Fe}_3\text{O}_4@\text{TiO}_2$ rapidly generates reactive oxygen species (ROS). Therefore, the detection methods and generation mechanisms of the intrinsic reactive oxygen species (ROS), as for instance superoxide anion radical ($\cdot\text{O}^{2-}$), hydrogen peroxide (H_2O_2), singlet oxygen ($^1\text{O}_2$), and hydroxyl radical ($\cdot\text{OH}$) in photocatalysis, were comprehensively surveyed.

Poster Presentation : **MAT.P-330**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Effect of Intercalated various alkylamines of 1T'-MoS₂ for Hydrogen Evolution Reaction

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The imminent global energy crisis and current environmental issues have stimulated considerable research on high-performance catalysts for sustainable hydrogen energy generation. Two-dimensional layered MoS₂ has recently drawn worldwide attention because of its excellent catalytic properties for the hydrogen evolution reaction (HER). In the present work, we prepared nitrogen (N)-rich 1T' (distorted 1T) phase MoS₂ layered nanostructures using different alkyl amines with 1–4 nitrogen atoms (methylamine, ethylenediamine, diethylenetriamine, and triethylenetetramine) as intercalants. The amine molecules intercalate at 10 atomic%, and simultaneously supply the N atoms that substitute the S atoms to produce the N-doped MoS₂, whose composition is MoS₂(1-x)N_x, where x = 0.1–0.26. MoS₂ prepared with amines having more N atoms has enhanced catalytic HER performance: a Tafel slope of 36 mV dec⁻¹ and 10 mA cm⁻² at -160 mV (vs. RHE). First-principles calculations showed that the amine intercalation and N doping increase the density of states near the Fermi level in a narrow range and bring about an effective overlap of the d_{z²}(Mo), p_z(S), and p_z(N) states. These factors in turn increase the carrier (electron) concentration and mobility for improved HER. The calculation also predicted that the most active site is S vacancies. The present work illustrates how the HER catalytic performance of 1T' phase MoS₂ can be effectively controlled by the amine molecules.

Poster Presentation : **MAT.P-331**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Nickel Phosphide Polymorphs with Active (001) Surface as Excellent Catalysts for Water Splitting

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Since the emergence of hydrogen generation by water-splitting as a core renewable-energy technology, the development of related catalysts with high efficiency, long-term stability, and low costs has been vigorously pursued. We report the temperature-controlled synthesis of two nickel phosphide polymorphs, Ni₂P and Ni₅P₄, by phosphorization of Ni foil or foams using phosphine gas. The hexagonal phase Ni₂P nanowires and Ni₅P₄ nanosheets were grown on Ni substrates with vertical alignment, and uniformly exposed active (001) planes. The Ni₅P₄ nanosheets possess significant stacking faults along the [0001] direction. Both Ni₂P and Ni₅P₄ exhibit excellent electrocatalytic activity toward the hydrogen evolution reaction (HER). Their overpotential for 10 mA cm⁻² was 0.126 and 0.114 V, and the Tafel slope was 42 and 34 mV dec⁻¹ in 0.5 M H₂SO₄ electrolyte, respectively. A decrease in HER performance was observed for Ni₅P₄, but the change was negligible for Ni₂P. Strain mapping using a precession-assisted nanobeam electron diffraction technique showed that only Ni₅P₄ underwent degradation of basal (001) planes during HER, which explains the lower stability of catalytic activity. Furthermore, the Ni₂P nanowires demonstrated excellent catalytic activity toward overall water splitting, which could be attributed to the stable surface as well as the highly conductive crystal structures.

Poster Presentation : **MAT.P-332**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Electrochemical Conversion of CO₂ into Various Products Using ZnO-Based Nanoparticles

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Increasing level of CO₂ concentration from the use of fossil fuels has become the most serious environmental concern related to global warming and climate change. The electrochemical CO₂ reduction reaction (CO₂RR) is a key reaction for CO₂ conversion to valuable fuels and chemicals. In this work, we report zinc oxide (ZnO)-based composite nanoparticles as a low-cost high-efficiency CO₂RR catalyst. They were synthesized by sol-gel method, followed by the annealing process. The composition control of ZnO-based nanoparticles results in more than 80 % Faradaic efficiency of CO₂ conversion either to CO or HCOOH with high selectivity. In order to understand the remarkable catalytic efficiency, the electronic structures were thoroughly investigated using synchrotron X-ray photoelectron spectroscopy and extended X-ray absorption fine structures, in combination with various electrochemical analyses.

Poster Presentation : **MAT.P-333**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Two Dimensional MoS₂ Meets Porphyrin via Intercalation: Phase Conversion to 1T' to Enhance Catalytic Activity Toward Hydrogen Evolution

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The intercalation of porphyrin molecules between MoS₂ layers was found to efficiently induce the phase conversion to 1T' MoS₂. The Mn-porphyrin is intercalated preferentially with the Mn(III) cations. The resultant Mn-porphyrin-MoS₂ exhibit excellent catalytic activity toward the hydrogen evolution reaction, with a Tafel slope of 35 mV dec⁻¹ and 10 mA cm⁻² at an overpotential of 0.125 V. Spin-polarized density functional theory calculations confirmed that the intercalation of Mn-porphyrin into 1T' MoS₂ is quite favorable due to strong charge transfer. In the Volmer reaction step, the active sites are identified as S atoms of MoS₂ located just above the Mn center.

Poster Presentation : **MAT.P-334**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Polytypic GaP and GaAs Nanowires and Application as Photodetectors

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One-dimensional semiconductor nanowires often contain polytypic structures owing to the co-existence of different crystal phase. Therefore, the understanding the properties of polytypic structures is of paramount importance for many promising applications in high-performance nanodevice. Herein, we synthesized typical III-V semiconductors, gallium phosphide (GaP) and gallium arsenide (GaAs), nanowires with zinc blende phase using the chemical vapor transport method. The growth direction ([111] and [211]) was controlled by the growth condition such as hydrogen gas flow. Various typed polytypic structures were produced simultaneously in a controlled manner. Nanobeam electron diffraction technique was employed to obtain strain mapping of the nanowires, which visualizes the polytypic structures along the [111] direction. We collected micro-Raman spectrum for individual nanowire, confirming the presence of hexagonal wurtzite phase in the polytypic nanowires. Further, we fabricated photodetectors using single nanowire, showing that the polytypic structures can decrease the photosensitivity. Our systematic analysis provides important insight into polytypic structures of nanowires.

Poster Presentation : **MAT.P-335**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Orthorhombic NiSe₂ Nanocrystals on Si Nanowires for Efficient Photoelectrochemical Water Splitting

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Photocatalytic water splitting is a vital technology for clean renewable energy. Despite enormous progress, the search for earth-abundant photocatalysts with long-term stability and high catalytic activity is still an important issue. We report three possible polymorphs of nickel selenide (orthorhombic phase NiSe₂, cubic phase NiSe₂, and hexagonal phase NiSe) as bifunctional catalysts for water-splitting photoelectrochemical (PEC) cells. Photocathodes or photoanodes were fabricated by depositing the nickel selenide nanocrystals onto p- or n-type Si nanowire arrays. Detailed structure analysis reveals that compared to the other two types, the orthorhombic NiSe₂ nanocrystals are more metallic and form less surface oxides. As a result, the orthorhombic NiSe₂ nanocrystals significantly enhanced the performance of water-splitting PEC cells by increasing the photocurrents and shifting the onset potentials. The high photocurrent is ascribed to the excellent catalytic activity toward water splitting, resulting in a low charge transfer resistance. The onset potential shift can be determined by the shift of the flat-band potential. A large band bending occurs at the electrolyte interface, so that photoelectrons or photoholes are efficiently generated to accelerate the photocatalytic reaction at the active sites of orthorhombic NiSe₂. The remarkable bifunctional photocatalytic activity of orthorhombic NiSe₂ promises efficient PEC water-splitting.

Poster Presentation : **MAT.P-336**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Two-dimensional Transition Dichalcogenide Nanosheets for Photoelectrochemical Hydrogen Production.

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Photocatalysts for hydrogen evolution reactions (HER) are central to key renewable energy technologies of water splitting. Despite tremendous effort, the development of low-cost electrode catalysts with high activity remains a great challenge. In this study, we report the transition metal dichalcogenide (TMD) layered two-dimensional (2D) nanosheets as excellent photocatalysts for water-splitting reactions. We fabricated a Si-based photocathode by depositing the TMDs nanosheets such as MoS₂, MoSe₂, MoTe₂, etc., onto an p-type Si nanowire array, showing efficient photoelectrochemical (PEC) hydrogen evolution under visible light irradiation. Band alignment suggested that the efficiency of the PEC cell is ascribed to the buildup of the space charge region in the heterojunction, as well as the band bending of Si at the electrolyte interface.

Poster Presentation : **MAT.P-337**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Two-Dimensional GeAs with Visible Range Band Gap

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Two-dimensional (2D) layered structures have recently drawn worldwide attention because of their intriguing optical and electrical properties. In this study, we prepared GeAs nanosheets as a new 2D material by a liquid-phase exfoliation method. The few-layered nanosheets had a band gap close to 2.1 eV, which is significantly higher (by about 1.5 eV) compared to the bulk. The value of 2.1 eV is in excellent agreement with that for the monolayer obtained from first-principles (HSE-06) calculations; mono-, bi-, and tri-, and tetralayers have remarkably direct or quasi direct band gap of 2.125, 1.339, 1.112, and 1.017 eV, respectively. The electrical properties of individual GeAs nanosheets were measured to reveal the 2D carrier transport behaviors. We also observed stable and large photocurrents, indicating potential application in high-performance optoelectronic nanodevices. The few-layered GeAs nanosheets deposited on n-type Si nanowire arrays showed promising photoelectrochemical water splitting under visible light irradiation. Band alignment based on the calculated band edge positions suggested a buildup of the space charge region in the p-GeAs/n-Si heterojunction, as well as the band bending of n-Si at the electrolyte interface

Poster Presentation : **MAT.P-338**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Strain Mapping of Bent III-V Semiconductor Nanowires

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Strain engineering of nanowires (NWs) has been recognized as a powerful strategy for tuning the optical and electronic properties of nanoscale semiconductors. Therefore, the characterization of the strains with nanometer-scale spatial resolution is of great importance for various promising applications. In the present work, we synthesized single-crystalline GaN, GaP, and GaAs nanowires using the chemical vapor transport method and visualized their bending strains (up to 3%) with high precision using the nanobeam electron diffraction technique. The strain mapping at all crystallographic axes revealed that maximum strain exists along the growth direction with the tensile and compressive strains at the outer and inner parts, respectively; the opposite strains appeared along the perpendicular direction; the tensile strain was larger than the coexisting compressive strain at all axes. These results are consistent with the mechanical modulus of bulk phase. Our work provides new insight into the bending strain of III-V semiconductors, which is of paramount importance in the performance of flexible or bendable electronics.

Poster Presentation : **MAT.P-339**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Controlled Assembly of Core-Shell Silica Microspheres for Photonic Crystals

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We report on an efficient and reproducible approach to make photonic crystals on the basis of monodisperse core-shell silica (SiO_2) microspheres. Diluted solution of silica seeds having an average diameter of about 40 nm was prepared by modified Stöber method, which was used as seeds for growing silica microspheres. Diameters of produced silica microspheres (core- SiO_2) are ranged ranging from 75 to 340, which can be synthesized by adjusting the amount of silica precursors. Silica shells were coated on core- SiO_2 microspheres by hydrolysis and condensation reactions of tetraethyl orthosilicate and octadecyl trimethoxysilane. Calcination of the coated SiO_2 microspheres in air rendered the core-shell silica (CS- SiO_2) microspheres. This size-controllable process allows large-scale synthesis of CS- SiO_2 . They are highly porous and monodisperse, and thus can be used as close-packed photonic crystal systems. We found that this colloidal assembly approach represents a simple and scalable method for generating high-quality photonic crystals.

Poster Presentation : **MAT.P-340**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Porous carbons derived from metal azolate framework-6: Preparation via pyrolysis and application in adsorptive removal of pharmaceutical and personal care products from water

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Porous carbons have been very useful in versatile applications in various fields, and several precursors were used for such carbons. Recently metal-organic frameworks (MOFs) are also widely used as precursors for porous carbons. In this study, porous carbons were obtained by high temperature pyrolysis of metal azolate framework-6 (a subclass of MOFs), especially in the co-presence of KOH activator. The porosity and defect concentration of carbon increased by adding KOH activator; and therefore, the obtained carbon might be very useful in adsorptions. Actually the carbons obtained in suitable condition showed huge adsorption capacity for wide range of pharmaceutical and personal care products (such as acidic ibuprofen; weakly acidic triclosan and oxybenzone; and basic diclofenac sodium and atenolol). A plausible adsorption mechanism for ibuprofen could be also suggested by adsorption in wide pH conditions. Moreover, the used carbon could be recycled easily by solvent washing. Therefore, metal azolate framework-6-derived carbon (especially in the co-presence of KOH activator) could be suggested as a potential adsorbent to purify water contaminated with organics such as pharmaceutical and personal care products.

Poster Presentation : **MAT.P-341**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Highly stable ionic liquid@MIL-101(Cr) adsorbents for the removal of benzothiophene from liquid fuel

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Recently, there is a considerable demand to reduce the content of sulfur and nitrogen containing organic compounds in fuels like diesel and gasoline to a very low level to prevent air pollution and deactivation of catalysts. Metal-organic frameworks (MOFs) modified with the introduction of acidic ionic liquids (ILs) have been employed to the adsorptive removal of benzothiophene (BT) from n-octane. ILs were synthesized inside a porous MIL-101(Cr) via a ship-in-bottle (SIB) technique. The maximum adsorption capacities (Q₀) for the virgin MIL-101(Cr) and for IL@MIL-101(Cr) were 49 and 68 mg/g, respectively, corresponding to a 37% increase in Q₀. The Q₀ value, based on the surface area (mg/m²) of the adsorbents, increased by 94% for ILs@MIL-101(Cr) (prepared via the SIB route), thus demonstrating the high affinity of ILs for BT. The improved adsorptive performance for BT might be derived from a specific interaction between the acidic ILs and the BT molecules. More importantly, unlike previously reported IL-incorporated MIL-101(Cr)s, IL@MIL-101(Cr) prepared by the SIB approach was very stable for adsorption of BT over several cycles.

Poster Presentation : **MAT.P-342**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Polyaniline-derived porous carbons: Adsorbent with record high adsorption capacities for the removal of personal care products from water

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Because of increasing living standard, huge production/consumption of PCPs and increasing population, contamination of water resources with personal care products (PCPs) is severe in recent days. In this study, removal of three typical PCPs such as triclosan, oxybenzone, and chloroxylenol was carried out via adsorption over highly porous carbon, prepared from pyrolysis of poly-amine under suitable condition. The carbons (named PDCs) showed record high adsorptions for the three PCPs. Moreover, the adsorption mechanism could be suggested by adsorptions in wide range of pH conditions. Or, H-bonding (PCPs as H-donor) might be the main mechanism to explain the remarkable adsorption. Additionally, the used PDC could be recycled by simple solvent washing. Therefore, the PDCs could be suggested as a potential adsorbent to adsorb/purify contaminated water with PCPs. Keywords: adsorption; polyaniline-derived porous carbon; personal care products; water purification.

Poster Presentation : **MAT.P-343**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Syntheses and applications of hydrophobic cobalt–azolate frameworks for water purification

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Two cobalt–azolate frameworks (MAF-5(Co) and MAF-6(Co)) with high porosity were synthesized in pure-phase at room temperature. The MAF-5(Co) and MAF-6(Co) are isostructural with MAF-5(Zn) and MAF-6(Zn) that was reported previously. For mixing the precursors for the MAFs were done in two different ways, e. g. slow and fast mixing method. Fast mixing method was observed as the most efficient method for synthesizing MAF(Co) materials in pure-phase with high yield. To characterize the obtained materials XRD patterns, N₂-isotherms, SEM-images, water and n-octane adsorption analyses were conducted. The synthesized MAFs(Co) high porosity and hydrophobicity, similar to the analogous MAFs those composed of Zn. To find the applicability of newly developed materials, MAF-5(Co) and MAF-6(Co), they were applied in the adsorption of n-octane as a model oil from water and the obtained results were compared to those of related materials, i.e., MAF-4(Co and Zn), MAF-5(Zn), and MAF-6(Zn), as well as with Cu-BTC (Cu-benzenetricarboxylate) together with a conventional adsorbent, activated carbon. Surprisingly, MAF-5(Co), even with low porosity, showed remarkable competitiveness among the typical porous materials for n-octane removal. However, better performance of MAF-6(Co) was observed for the adsorption of n-dodecane. The obtained results suggested that the framework structure including cavity and aperture sizes rather than surface area play a critical role in the hydrocarbon (n-octane or n-dodecane) removal from water. Moreover, simple evaporation of the adsorbed n-octane was enough to regenerate the adsorbent MAF-5(Co) for next uses and thereby suggested as a potential adsorbent for the removal of spilled oil from water. Therefore, the synthesized MAFs can be suggested as impressive adsorbents in water purification probably on account of their hydrophobicity.

Poster Presentation : **MAT.P-344**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of SSZ-13 zeolite in the presence of dimethylethylcyclohexyl ammonium (DMCHA) ion and application of SSZ-13 in direct conversion of ethylene to propylene

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The conversion of Y zeolites (in the absence of any seed) having wide silica/alumina ratio (SAR, 5.1–80) into SSZ-13s was carried out in the presence of N,N,N-dimethylethylcyclohexylammonium (DMCHA) ion, as an organic structure directing agent (OSDA). Analcime or analcite phase (ANA) was obtained in case of low SARs (5.1 and 12) of the starting Y zeolites. Sodium silicate was used to increase the SARs of Y zeolites and played a vital role for the successful conversion of low SARs (5.1 and 12) Y zeolites. The protonated SSZ-13 zeolites with wide SAR ranges were employed in the direct ethylene-to-propylene (ETP) conversion to investigate not only the effect of the SARs on the ETP reaction but also the conversion of ethylene with propylene selectivity. The results showed that the SSZ-13s with moderate SARs have better catalytic activity than SSZ-13s with lower and higher SAR values. Moreover, DMCHA-Br derived SSZ-13 was better or quite competitive in ETP against SSZ-13 synthesized by using tetraethylammonium hydroxide as OSDA. Therefore, DMCHA⁺ can be recommended as a versatile OSDA for the conversion of Y zeolites into SSZ-13 based on low cost, and applicable for wide SAR range of starting Y zeolites as well as excellent performance in ETP reaction.

Poster Presentation : **MAT.P-345**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Highly stable superhydrophobic film surface by a facile UV process at room temperature

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Preparation of superhydrophobic, transparent and highly stable film at room temperature by a facile UV process. In this experiment, we can get transparent, hydrophobic and high stable film by UV process at room temperature(RT). We synthesized a material by thiol-ene click reaction between V-POSS and -SH under UV radiation at RT. The vinyl, functional groups, was substituted with octadecanethiol and 1,10-decanedithiol. After spray coating with made material, the film showed superhydrophobicity by substitution with octadecanethiol and high stability by substitution with 1,10-decanedithiol. The resulting film result in a water contact angle greater than 150° and a small sliding angle ($SA \leq 10^\circ$). In addition, the coated surfaces still retained the superhydrophobicity after sonication.

Poster Presentation : **MAT.P-346**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Solution-Processed High-k Dielectrics by Sol-Gel Dip-Coating Method for Thin-Film Transistors

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Recently, it reported on high-k dielectric via spin-coating method. In this study, we had demonstrated a solution-processed high-k dielectric material via sol-gel dip-coating method. These film are fabricated via solution processes and had a lower gate leakage current density than a film via spin-coating method. Thin-film transistors fabricated with organic and inorganic semiconductors exhibited high mobility and current on-off ratios. Also, these devices function well at low voltages.

Poster Presentation : **MAT.P-347**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

One-Step Fabrication of Hydrophobic Hybrid Gate Dielectrics for Low-Voltage Organic Thin-Film Transistors

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We demonstrate the design, processing, and dielectric properties of low surface energy organic/inorganic hybrid dielectric films for low-voltage operation of organic thin-film transistors (OTFTs). The hydrophobic hybrid dielectric films are easily fabricated by one-step spin coating of a zirconium chloride precursor in an octadecyltrimethoxysilane solution under ambient conditions, followed by thermal curing at low temperatures (approximately 150 °C). These novel dielectrics exhibit excellent surface smoothness (rootmean-square roughness is

Poster Presentation : **MAT.P-348**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Multifunctional Hybrid Nanomaterials for Highly Flexible and Self-Healable Superhydrophobic Films

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For constructing bio-inspired functional films with various superhydrophobic functions including self-cleaning, anti-corrosion, anti-bioadhesion, and oil-water separation, hydrophobic nanomaterials have been widely used as crucial structural components. In general, hydrophobic nanomaterials, however, cannot form strong chemical bond networks in organic-inorganic hybrid composite films because of the absence of chemically compatible binding components. Herein, we report bio-inspired design and synthesis of multifunctional hybrid nanomaterials with tunable functionalities of covalent cross-linking and hydrophobicity for constructing three-dimensionally interconnected superhydrophobic composite films via a facile solution-based fabrication at room temperature. The multifunctional hybrid nanomaterials allow the systematic control of functionalities of composite films, as well as the stable formation of covalently linked superhydrophobic composite films with excellent flexibility (a bending radius of 6.5mm, 1000cycles) and self-healing ability (water contact angle $> 150^\circ$, ≥ 10 cycles). The presented strategy can be a versatile and effective route to generating other advanced functional films with covalently interconnected composite networks.

Poster Presentation : **MAT.P-349**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Study on thin film transistor (TFT) characteristics for biosensor application

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Recently, studies for developing advanced biosensors have been made to prevent diseases with latent period such as avian influenza or mers virus. Among various type of biosensor, TFT-based biosensors have attracted great interests in developing. The advantages of TFT-based biosensor are high sensitivity, low cost, easy fabrication and flexibility. However, TFT-based biosensors still have limitations due to their unstable properties for environmental factors such as water and air. Therefore, we have studied the properties of TFT under different environment conditions to developing TFT-based biosensors.

Poster Presentation : **MAT.P-350**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of mesoporous molybdenum disulfide with double-gyroid structure and Comparison in reaction pathway of bulk and nano-sized molybdenum disulfide

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MoS₂ has superior electrochemical properties suitable for lithium ion battery, such as high theoretical capacity (670 mAh/g), low volumetric expansion during cycle (~103%) and the weak *vdw* forces between layers, which enables facile intercalation/deintercalation of Li⁺. The lithium storage mechanism of MoS₂ is widely known as an irreversible intercalation reaction in the first cycle and a reversible conversion reaction (MoS₂ + 4Li⁺ + 4e⁻ ↔ Mo + 2Li₂S). However, there are some recent studies that contradict above mentioned mechanism and suggesting different reversible reaction path (Li₂S ↔ 2Li⁺ + S²⁻), similar to a lithium-sulfur battery reaction. In order to clarify the lithium storage mechanism of MoS₂, we first synthesized ordered mesoporous MoS₂ as a model structure to ascertain the complete mechanism by obtaining the maximum reversible capacity from this material. We utilized synchrotron radiation based characterization techniques to directly observe the local and bulk structural changes in the well-synthesized mesoporous MoS₂ model material during the electrochemical cycling. The oxidation state changes of Mo and S were observed during the 1st irreversible and 2nd reversible electrochemical cycle using XAS and XPS. The in situ XRD experiment was used to confirm the formation of Li₂S and/or Mo metal during the reversible reaction. In addition, SAXS was also used to observe the pore structure dynamics during the cycling of mesoporous MoS₂ electrode.

Poster Presentation : **MAT.P-351**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Hard templating synthesis of core-shell type mesoporous carbon and its application

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The rechargeable batteries are in high demand to address increasing electric devices market. Li-ion batteries get the possession because of its high energy density and lightness, but it's hard to use for electric vehicles and ESS due to its low capacity. So many researches are under way for alternative batteries. Among them, Li-S batteries have attracted much attention for it has high capacity and use low-cost active materials compared to Li-ion batteries. However the active material, sulfur dissolves as polysulfides intermediates while charging and discharging. This makes the capacity decrease and followed by poor cycle performance. So we tried to design new cathode materials that can block the elution of polysulfides by making microporous carbon layer. In our study, we synthesized phosphorus ordered meso-microporous carbon by nanocasting and coating method. Rod-type SBA-15 silica was used as hard template. Herein, we controlled the amount of phosphoric acid and thickness of coated carbon. The as-synthesized materials were characterized by X-ray diffraction(XRD), N₂-sorption isotherm and scanning electron microscope(SEM).

Poster Presentation : **MAT.P-352**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Metal Organic Framework with Omni-Valent Cation Storage for Fast and Charge-Efficient Ion Removal of Capacitive Deionization

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Capacitive deionization (CDI) that engages porous carbon electrodes is one of the well-established energy-efficient desalination techniques. Nevertheless, the desalination performance such as ion removal capacity and charge efficiency is still limited due to the reverse adsorption of co-ions, which occurs to meet charge neutrality. Herein, an asymmetric CDI is introduced by pairing metal organic framework (MOF) and porous carbon electrodes. The exclusive intercalation of cations into the MOF prevents the reverse adsorption of co-ions (anions), thus significantly improving ion removal capacity (23.2 mg g^{-1}) and charge efficiency (75.8%). Besides, diverse monovalent and divalent cations can be captured into the A sites of the MOF at similar redox potentials. Moreover, cations are intercalated in the hydrated forms, facilitating fast desalination by reducing the desolvation energy penalty at the electrode-water interface. The asymmetric CDI also exhibits voltage-insensitive deionization behavior and keeps pH within the limited range. This study offers a new design principle in CDI, that is, the integration of a crystal structure with large ionic channels that enable the hydrated intercalation of ions in a fast and exclusive manner.

Poster Presentation : **MAT.P-353**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Antiplaetlet coating with poly((3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide) on titanium dioxide and stainless steel

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When medical devices such as stent and catheter are inserted in blood vessel, platelet adhesion can cause a serious problem like blood coagulation, resulting in vascular clogging. To inhibit platelet adhesion on medical devices, in this work, we employed a zwitterionic material, (3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide (MPDSAH) by considering that zwitterionic polymers have antifouling effects by strongly stabilizing the hydration layer formed by aqueous solution. Titanium dioxide (TiO₂) and stainless steel (SS), which are mainly used in medical devices, were chemically modified by surface-initiated atom transfer radical polymerization of MPDSAH. The surface-grafted polymeric films were characterized with ellipsometer, contact angle goniometer, X-ray photoelectron spectroscopy, and atomic force microscopy. Compared with bare substrates, the poly(MPDSAH)-coated substrates effectively reduced both fibrinogen and platelet adhesions. The platelet adhesion was reduced by 86% and 92% for the polymer-coated TiO₂ and SS substrates, respectively.

Poster Presentation : **MAT.P-354**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Phase-Selective Synthesis of Two-Dimensional MoTe₂ through Te Flux Control

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To realize high-performance two-dimensional electronics, it is necessary to form two-dimensional metal-semiconductor junctions with minimized contact resistance. We have developed a chemical method of selectively achieving semiconducting 2H MoTe₂ and metallic 1T' MoTe₂ by adjusting Te flux. Molybdenum nanoislands were formed on a substrate by electron-beam evaporation, and then they were tellurized with appropriate Te flux to selectively synthesize 2H MoTe₂ and 1T' MoTe₂. By combining this new phase-selective synthetic strategy with a lithographic technique, in-plane two-dimensional metal-semiconductor junctions composed of the same material can be formed in a selected pattern on the substrate. This method could be utilized for the mass production of high-performance electronic devices based on two-dimensional materials.

Poster Presentation : **MAT.P-355**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of lithium hydroxides layers on aluminum metal foils

Yongju Lee, Duk-Young Jung*

Department of Chemistry, Sungkyunkwan University, Korea

An LiAl₂-layered double hydroxide(LDH) was synthesized on an aluminum foil in an aqueous solution of LiCl by urea hydrolysis to adsorb lithium cations. As-adsorbed lithium cations in LiAl₂-LDH were simply extracted in a distilled water at 70~90 °C. This work presents a method for directly growing oriented LiAl₂-LDH films on aluminum foil. The concentrations of urea and LiCl were controlled to find the optimal conditions for synthesis of LiAl₂-LDH. The concentration of LiCl is a critical factor rather than the concentration of urea in the synthesis of LDH. Concentration of as-adsorbed lithium cations in LiAl₂-LDH was determined by inductively coupled plasma(ICP), thermogravimetric analysis(TGA) and lithium ion selective electrode(ISE).

Poster Presentation : **MAT.P-356**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of new lead bromide perovskite single crystal

Eunji Lee, Ji-Hyun Cha, HyunJong Lee, Duk-Young Jung*

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Organic-inorganic halide perovskite single crystals have received enormous amount of attention because of their exceptional optical and electronic properties with useful optoelectronic applications. Appropriate organic and inorganic compounds can be applied to form diverse chemical structures of this type material. Synthesis of hybrid perovskite single crystals with various organic components is essential to investigate the relationship between chemical structures and optoelectronic property of the crystal. Herein, the synthesis and characterization of lead bromide perovskite single crystal with a new organic cation is investigated. Colorless and transparent single crystal grows by solution growth processes. Chemical structure of perovskite crystals were determined by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), energy dispersive x-ray spectroscopy (EDS) and thermogravimetric-differential thermal analysis (TG-DTA).

Poster Presentation : **MAT.P-357**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Copper-indium and Copper-gallium diethyldithiocarbamate complexes

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Copper(III) diethyldithiocarbamate(dtc) complexes $[\text{Cu}(\eta^2\text{-S}_2\text{CNEt}_2)_2][\text{InCl}_4]$ and $[\text{Cu}(\eta^2\text{-S}_2\text{CNEt}_2)_2][\text{GaCl}_4]$ have been synthesized and characterized as precursors of CIGS thin film. These compounds were synthesized by using Cu(II)-dtc, In(III) chloride and Ga(III) iodide in dichloromethane and ethanol. Particularly, Ga(III) iodide reacts with iodine-chlorine substitution reaction in dichloromethane. Cu(III)(ddtc) $^{2+}$ cation contain square-planar Cu(III) centres which attain on overall distorted octahedral coordination environment with long range intermolecular interactions between copper-sulfur. In $[\text{Cu}(\eta^2\text{-S}_2\text{CNEt}_2)_2][\text{MeCl}_4]$ (Me = In, Ga), anions and cations do not interact and both compounds have same crystal packing system. Crystal structures of both compounds have been determined by single-crystal X-ray diffractometer. Modification of molecular system of Cu-dtc was investigated by measurement of IR. TGA was utilized to analyze melting point of them to study the thermal reaction condition for fabrication of CIGS thin films of photovoltaic device

Poster Presentation : **MAT.P-358**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Carbon Materials with Porosity and Metal Nanoparticles for Shuttle Effects

Ye Lim Kwon, Min Ji Kim, Ji Man Kim*

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Secondary batteries are becoming important with increased use of portable electronic devices. Li-ion battery is the most commonly used but it has some problems like explosion and high price. Li-S battery is a one of the promising alternative to Li-ion battery. It has high theoretical energy density, low cost, eco-friendliness and safety. But polysulfide anions are dissolved in the repetitive charging and discharging so it makes the capacity decrease, which is called shuttle effect. To minimize shuttle effect, we modified ordered mesoporous carbon(OMC) materials. OMC has high thermal and chemical stability, high surface area and high pore volume. We synthesized the OMC materials with micropores by introducing silica nanoparticles and loaded metal nanoparticles on the OMC. 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-359**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Peapod-like Arrangement of Multicompositional Noble Metal Nanoparticles Embedded within Hollow Silica Nanotubes

Suncheol Kim, Hyojong Yoo*

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Nanoparticle assemblies within hollow nanoshells provide access into advanced nanohybrids with unique and colligative properties. Herein, a simple and effective solution-based synthetic approach for peapod-shaped Au nanoparticle assembly embedded within hollow silica nanotubes (pp multi-Au@SiO₂ NTs) is reported. Firstly, one-dimensional [multiple Au nanodot] core-[silica] shell nanowires (multi-Au@SiO₂ NWs) are synthesized using reverse microemulsion techniques. A subsequent thermal treatment of multi-Au@SiO₂ NWs in aqueous polyvinylpyrrolidone (PVP) solution results in the formation of pp multi-Au@SiO₂ NTs. Further overgrowth of secondary materials (i.e., Pt) on the Au nanoparticles in pp multi-Au@SiO₂ NTs results in the generation of [Au] core-[Pt] shell (Au/Pt) nanoparticle assemblies surrounded by silica nanotubes (pp multi-Au/Pt@SiO₂ NTs). The obtained one-dimensional nanoparticle assemblies encapsulated within hollow silica nanotubes can be efficient and selective nanoreactors for targeted catalysis.

Poster Presentation : **MAT.P-360**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Controllable Fabrication and Application of Dendritic Fibrous Nanosilica/Metallic Nanoparticles/Coordination Polymer Hybrid Nanomaterials

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The establishment of versatile and efficient strategies for the preparation of multicomponent nanohybrids with distinct functions are at the forefront of nano-engineering. In this work, dendritic fibrous nanosilica (DFNS) with excellent hydrothermal, mechanical stabilities and a high degree of porosity is successfully employed as a template to fabricate DFNS/metallic nanoparticles (NPs) hybrid nanomaterials. The NH₂-functionalized DFNS/metallic NPs hybrids subsequently employed as seeds to grow coordination polymer (CP) shells leads to the formation of DFNS/metalic NPs/CP core-shell nanohybrids. The obtained DFNS/metalic NPs/CP nanohybrids are promising to be used in a variety of applications. In addiiton, the as-synthesized DFNS/metalic NPs/CP nanohybrids can act as sacrificial templates for the unique inorganic hybrid nanomaterials via thermally-induced approaches.

Poster Presentation : **MAT.P-361**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Effective Encapsulation of Gold Multipod Nanoparticle Cores within ZIF-67 Shells Nanohybrids (GMN@ ZIF-67) with Structural Tunability

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¹*Chemistry, Hallym University, Korea*

Advanced hybrid nanomaterials tailored with unique morphologies and multiple functions can be fabricated by the rational combination of two or more well-designed components. Herein, gold multipod nanoparticle core–zeolitic imidazolate framework shell (GMN@ZIF-67) nanohybrids are successfully synthesized in an effective and scalable manner. Because of the structural anisotropy and uniqueness of GMNs, the formation of nanohybrids with ZIF-67 can be readily achieved without using any bifunctional ligands, surfactants, or other polymers, rendering it a potential use as environmentally-friendly method. The size of the GMN@ZIF-67 nanohybrids can be adjusted by either varying the molar ratio of ZIF-67 precursors or the quantity of GMNs used.

Poster Presentation : **MAT.P-362**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Controllable Synthesis of a Highly Ordered Polymeric Structure Assembled from Cobalt-Cluster-based Racemic Supramolecules

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Department of Chemistry, Hallym University, Korea

Metallosupramolecule-based polymeric architectures with high degrees of hierarchy and tailorable functionalities are interesting due to their unique morphologies and potential applications. Herein, the controllable synthesis of a highly-ordered polymeric structure, $\{[M,P-Co_8(PDA)_6(HIP)_3(DMF)_5(H_2O)]_3-[Co(DMF)(H_2O)_2]\}$ (1) (PDA = 2,6-pyridinedicarboxylate, HIP = 5-hydroxyisophthalate, DMF = dimethylformamide) with unique topology is reported. The solid-state structure of 1 reveals that it is alternately and periodically assembled from racemic supramolecular monomers to form a zigzag-shaped polymeric strand. Discrete racemic supramolecules (2) with topologies similar to those of monomeric species of 1 are also controllably synthesized in a separate reaction. Formation of intermolecular hydrogen bonds between supramolecules associated with hydroxyl groups of HIPs are critical for the unique solid-state packing geometries of 1 and 2.

Poster Presentation : **MAT.P-363**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Controllable Synthesis and Application of Dendritic Fibrous Nanosilica (DFNS)/Gold (Au) Hybrid Nanomaterials

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Department of Chemistry, Hallym University, Korea

Dendritic fibrous nanosilica (DFNS) with a high surface area is successfully employed as a template to synthesize DFNS/Au hybrid nanomaterials. Au nanodots are initially synthesized by the selective reduction of Au ion on the surface of the DFNS after surface modification to form DFNS/Au dots. A seed-mediated growth method is used to controllably grow Au nanoparticles on the DFNS/Au dots to generate DFNS core-Au NPs shell nanoparticles (DFNS/Au NPs) and DFNS core-Au layer shell nanoparticles (DFNS/Au layers). The catalytic activities of DFNS/Au NPs and DFNS/Au layers in the 4-nitrophenol reduction reaction are compared.

Poster Presentation : **MAT.P-364**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Facile Synthesis of Coordination Polymer Nanocubes and Post-Modification through Secondary Metal Ion Decoration

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Coordination polymer particles (CPPs) are generally formed through the coordination-driven assembly of metal ions or clusters with multitopic organic linkers. Their high degree of porosity, well-defined pore size, and structural tailorability render them promising candidates for diverse applications. Herein, we report a shape-controllable synthetic protocol for Zinc-based coordination polymer nanocubes (Zn-CPNs). In the synthesis, 2,6-bis[(4-carboxyanilino)carbonyl] pyridine ([N3]) ligand is employed as an efficient shape-directing modulator to control the size and shape of Zn-CPNs. More importantly, the Zn-CPNs provide plenty of metal binding sites and beneficial defects in the structure, which is suitable for the coordination of other functional metal ions. The secondary metal ion-modified Zn-CPNs exhibit improved catalytic activities.

Poster Presentation : **MAT.P-365**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Integration of Fluorescent and Magnetic Properties within Silica Hybrid Nanosystems

So Eun Jung, Hien Duy Mai, Hyojong Yoo*

Department of Chemistry, Hallym University, Korea

Iron oxide nanoparticle cores - silica shell nanostructures with multi-functional properties are successfully fabricated in a facile and high-yielding manner. The sodium oleate-modified Fe₃O₄ nanoparticles (NPs) are effectively encapsulated within silica matrix through both Stöber and reverse-microemulsion (water-in-oil) methods. Both organic (fluorescein) and inorganic (RUBY) dyes are incorporated through the sequential hydrolysis and condensation of tetraethylorthosilicate (TEOS) and 3-(aminopropyl) triethoxysilane (APTES) to form highly fluorescent, multiple Fe₃O₄ nanoparticle core-silica shell nanoparticles (FL multi-Fe₃O₄@SiO₂ NPs). These approaches for multi-functional nanoparticles can be efficiently applied for the fabrication of interesting nanomaterials useful in a variety of areas.

Poster Presentation : **MAT.P-366**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Metallocavitand-Induced Cage-like Crystal Packing within High-Order Cobalt Cluster-based Supramolecular Assemblies

Philjae Kang, Hien Duy Mai, Hyojong Yoo*

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A cobalt (Co) supramolecular triple-stranded helicate, $[\text{Co}_8(\text{PDA})_6(\text{Br-PTA})_3(\text{DMF})_4(\text{H}_2\text{O})_2]$ (**1**) (PDA = 2,6-pyridinedicarboxylate, Br-PTA = 5-bromoisophthalate, DMF = dimethylformamide), is successfully synthesized and fully characterized. The solid-state structure of **1** shows that four cobalt atoms are coordinated by three PDA ligands to form a tetranuclear cobalt cluster with three extension points and the ditopic Br-PTA ligands interlink two basic assembly units. In crystal packing, the bromo group is surrounded by the cavity-like tetranuclear cobalt cluster, which acts as a metallocavitand, to generate a unique cage-like crystal packing geometry. The isomorphous molecular cage, which exhibits similar crystal-packing geometry as observed in **1**, is also successfully isolated. This is an unusual example of a highly symmetric cage-like crystal packing architecture, resulting from the interaction among metallocavitands of in-situ generated supramolecular modules.

Poster Presentation : **MAT.P-367**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Facile Fabrication of Heterometallic Nanostructures through a Controllable Growth of Palladium Shells onto Gold Multipod Nanoparticle Cores

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Heterometallic nanostructures, such as bimetallic core-shell nanostructures and alloy structures, have been extensively investigated due to their potential applications in many fields including catalysis, electronics, sensors, and biomedicine. Despite much advances in nano-engineering, the overgrowth of secondary materials onto pre-synthesized seeds in a controllable manner to form core-shell configurations are still practically challenging. Herein, we report a high yielding and facile fabrication of bimetallic nanostructures through the epitaxial or islanded overgrowth of Pd shells onto gold multipod nanoparticle core (GMN@Pd NPs). Such hybrid nanostructures with anisotropic components could lead to significantly enhanced physical and chemical properties due to the possible synergistic effect.

Poster Presentation : **MAT.P-368**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Metallosupramolecular Nanocages through the Assembly of Triple-Stranded Helicates.

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Hallym University, Vietnam

¹Department of Chemistry, Hallym University, Korea

Triple-stranded helicates-based metallosupramolecular nanocages are successfully synthesized through unique multiple assembly strategy. The prepared discrete molecular nanocages are considered the assembly of six triple-stranded helicates interconnected by four metallic junctions. These are unusual examples of a highly symmetric discrete molecular architectures, resulting from the coordination-driven assembly of in-situ generated modules. The right- and left-handed triple-stranded helicates, structurally analogous to the basic building blocks in molecular nanocages can be synthesized in separated reactions. Owing to the presence of structurally well-defined, highly systematic, and robust cavities of the synthesized cages, the molecular nanocage shows much higher CO₂ capture capacity and selectivity compared with the triple-stranded helicates and other single molecules.

Poster Presentation : **MAT.P-369**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Metal-ion Tuning in Amine-Functionalized Supramolecular Triple-Stranded Helicates and Their Higher-Order Polymeric Assemblies

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With respect to the design of metallosupramolecules, the choice of metal ions is of considerable importance for the targeted crystal structures. Herein, we report a strategy to achieve isostructural amine-functionalized supramolecules containing different transition metals (cobalt, nickel, and manganese), namely, $M_8(PDA)_6(AIP)_3(DMF)_6$, where M = Co (1), Ni (2), and Mn (3) (PDA = 2,6-pyridinedicarboxylate, AIP = 5-aminoisophthalate, DMF = dimethylformamide). The variation in the transition metal ions used negligibly affects the coordinative assembly of metal and ligand species, suggesting a high degree of symmetry and stability of triple-stranded helical conformations. In addition, the change in metal ions can lead to distinctive physical or chemical properties of the resultant TSHs. In addition, 1, 2, and 3 can be employed as conceptual supramolecular modules for the construction of higher-order polymeric structures via the coordination with extra metal ions.

Poster Presentation : **MAT.P-370**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

New approach for fabricating the controllable high-resolution nanostructures by the combination of secondary sputtering phenomenon and electroplating process .

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The development of large-area, high-resolution nanostructure patterning with high aspect ratios is a challenging problem that must be addressed for potential applications in high performance nanoscale devices, such as nanoelectronics, optics, microfluidics, organic solar cell, display devices and biosensing devices. We fabricated size-controllable 3D patterned nanostructures with a wide range of resolutions (from ten nanometers to a few hundreds of nanometers) and a high aspect ratio over a large area through controlled plasma ion reactions and an electroplating process. This technique can produce various 3D patterns with ultrahigh resolution by utilizing (i) secondary sputtering during the plasma ion process, which can enable the fabrication of 3D structures on the 10 nm scale, and (ii) finely controlled electroplating (square-pulse-mode electroplating), which can control the resolution of structures through simple solution reactions by increasing the thickness of the original 10 nm-scale SSL-derived structures. Additionally, this technique can be extended to produce features with various 3D shapes (lines, hole-cylinders) from various other conductive materials (Cu, Al, Ag, etc.) on various types of substrates (silicon wafers, transparent glass, and flexible PC films). Accordingly, this new lithographic technique can serve as a next-generation patterning method for fabricating complex high-aspect-ratio patterned structures with ultrahigh resolution.

Poster Presentation : **MAT.P-371**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

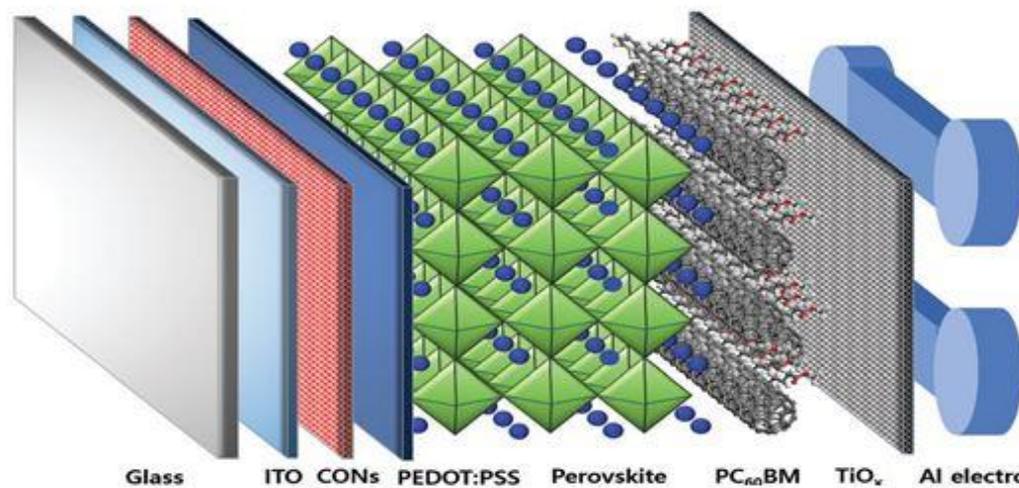
Covalent organic nanosheets for effective charge transport layers in planar-type perovskite solar cells

Kim Min-Sung, Jin Kuen Park*

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Solvent-treated bandgap-tunable covalent organic nanosheets (CONs) were prepared via the Stille cross-coupling reaction. These materials are considered useful as interlayers in photovoltaic devices upon the alignment of energy levels between other components. Among various types of solar cells, according to the organic-interlayer study, inverted planar perovskite solar cells (PSCs) are mostly demanded to effectively transport and collect charge carriers due to their high performance. As a result, the power conversion efficiencies (PCEs) of the optimized devices with CON-10 exhibited a value of 10.2%, which represented a 1% increase over those of the reference devices without the CONs and was 4% higher than that of the CON-16 devices. Moreover, the devices with CON-10 were further optimized with TiO_x using Al electrodes, leading to a PCE increase of these devices that became slightly higher than the PCEs of the device with CON-10 and without TiO_x. This tendency was supported by photoluminescence (PL) spectroscopy, photocurrent density (J_{ph}), and space-charge-limited current (SCLC) mobility results.

Figure 1. Schematic of the device architecture of the planar-type MAPbI₃ perovskite solar cells (PSCs) that were used in CONs.



Poster Presentation : **MAT.P-372**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Integration of heater and temperature sensor on paper-based DMF chip by using material inkjet printer

Yunpyo Kim, Veasna Soum, Mary Chuong, Sooyong Park, Oh-Sun Kwon*, Kwanwoo Shin*

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Integration of heaters and a temperature sensor on top of a digital microfluidic (DMF) paper-based lab-on-a-chip (p-chip) has been performed by using a simple printing technique. Behalf of advantages of printing technique, such as easy, quick and affordable deposition of materials on flexible paper, we can fabricate a film type of micro heater and temperature sensor to achieve an integrated p-chip. Firstly, by using an inkjet printer, Dimatix, silver nanoparticle (AgNP) ink was printed to obtain a rail pattern of guide electrodes, which was used for the dynamic actuation of DMF droplets driven by electrowetting force. Secondly, to provide a heat system on the p-chip surface, the AgNP ink was printed, forming a heat zone, which is composed of a pair of heaters enclosing a temperature sensor. The temperature sensor was a thermocouple type composed of the interfacial junction of overlapped layers of the thermoelectric (TE) material, p-type PEDOT:PSS over the metallic AgNP. The sensor showed a linear response with a Seebeck coefficient of 18.873 $\mu\text{V/K}$ in a range of 25 - 80 $^{\circ}\text{C}$, demonstrating good usage as a self-powered temperature sensor especially for a DMF drop with on-chip monitoring. This micro thin-film heating and sensing system embedded on p-chip enables us to manage not only the heating a droplet easily capable of the endothermic reaction, but also dynamic operations of droplet, such as merging, mixing and transporting. A biochemical experiment will be performed on this integrated heater-sensor DMF chip, promising a stand-alone portable chip for POC device which is an ultimate goal in this research. Keywords: Electrowetting, paper DMF, inkjet printing, Seebeck coefficient, heater, temperature sensor

Poster Presentation : **MAT.P-373**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Research on controlling the self-assemblies and optoelectronic properties of the organic semiconductors.

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For the research of organic semiconductors, we focused on Donor-acceptor oligomers. That is composed of four 2-Amino-7-bromofluorene (fluorene) as the electron donor and one perylene-3,4,9,10-tetra carboxylic dianhydride (perylene) as the electron acceptor. Final product can be used to fabricate a one-dimensional fibrillated optoelectronic device. Typically, Perylene bisimides (PBI) belong to a class of n-type chromophores exhibiting relatively high electron mobility, large molar absorption coefficients, fluorescence quantum yield, as well as good thermal and photochemical stabilities. Two fluorene and benzothiazole are synthesized by Suzuki coupling. A long chain is formed by attaching 6 alkyl chains on one side of fluorene, and it can be purified by chromatography. The long chain thus synthesized is a chromophore, which is attached to both side of perylene to synthesize N,N'-((7,7'-((1,3,8,10-tetraoxo-3,3a,7a,8-tetrahydroanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-2,9(1H,5aH,5bH,10H)-diyl)bis(9H-fluorene-7,2-diyl))bis(benzo[c][1,2,5]thiadiazole-7,4-diyl))bis(9H-fluorene-7,2-diyl))bis(3,4,5-tris(2,5,8,11,14,17-hexaoxonadecan-19-yloxy)benzamide) (P4F6A). Thus, the products allow for conjugation over a wider wavelength range. It is possible to conform π - π stackings of perylene and fluorene, that have more photochemical stability. Synthesized oligomers can be confirmed by NMR spectroscopy and MALDI-TOF. And, The photochemical properties can be confirmed by UV spectroscopy.

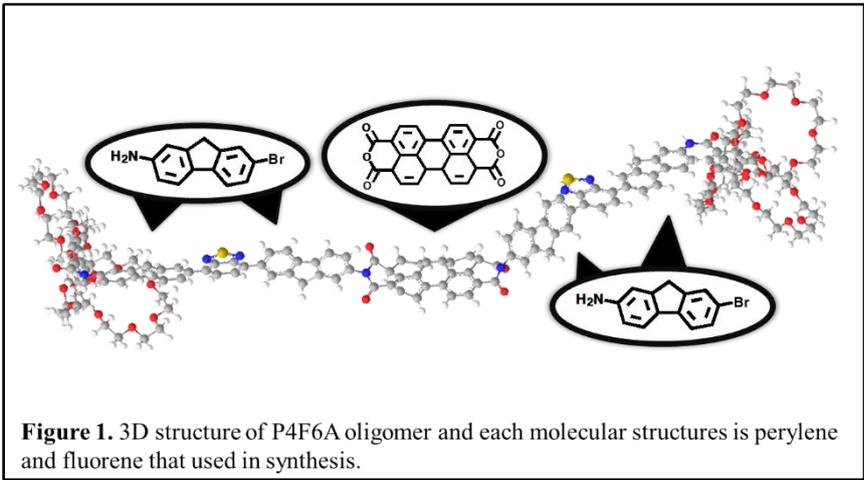


Figure 1. 3D structure of P4F6A oligomer and each molecular structures is perylene and fluorene that used in synthesis.

Poster Presentation : **MAT.P-374**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

High-Performance Iron Oxide-Based T2 MRI Nanoprobes in Ultra-High Magnetic Field

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To date, it has not been believed that superparamagnetic iron oxide (SPIO) nanoparticles (NPs) can offer improved performance in ultra-high magnetic field (UHF) MRI, because of their magnetization being saturated at low magnetic field. In this work, we provide a paradigm of hierarchical surface-structured, superparamagnetic (His) DyxFe_{3-x}O₄ NPs as a novel class of previously unexplored materials for superior T2 MRI nanoprobes at UHF (9.4 T). We found that His-DyxFe_{3-x}O₄ NPs ($x = 0.2$) possess a higher transverse relaxivity than unmodified His-SPIO NPs and a significantly enhanced r_2/r_1 ratio (up to ~10.4 times higher) than those of reported Dy-based T2 MRI probes at 9.4 T. Furthermore, we demonstrate the effects of surface design of DyxFe_{3-x}O₄ NPs on their magnetic relaxivity and in vivo performance at UHF. The markedly enhanced r_2/r_1 is attributed to the enhanced spin decoherence arising from the magnetic field inhomogeneity, as well as a freezing effect owing to stronger dipolar coupling of superparamagnetic His-DyxFe_{3-x}O₄ NPs ($x = 0.2$). Detailed experiment methods and results would be presented at this meeting.

Poster Presentation : **MAT.P-375**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Fabrication of Porous β -Bi₂O₃ Nanoplates and Their Enhanced Photocatalytic Activity and Capacitance Behavior

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Direct phase transformation of bismuth complex nanoplates to β -Bi₂O₃ ones was induced by low-temperature annealing at 250°C. The β -Bi₂O₃ nanoplates showed a nanoporous structure, which retained the tetragonal framework of the original bismuth complex nanoplates while releasing gas molecules produced during thermal decomposition, thereby enabling the formation of nanoporous structures extending through the nanoplate surfaces. The sizes, structures, optical properties, and composition distributions of the synthesized bismuth-organic complex and porous β -Bi₂O₃ nanoplates were characterized by scanning electron microscopy, energy-dispersive x-ray spectroscopy, infrared spectroscopy, UV-vis diffuse reflectance spectroscopy, and x-ray diffraction. The porous β -Bi₂O₃ nanoplates prepared by low-temperature annealing at 250°C for 3, 5, and 7 h showed photocatalytic activities for the photodegradation of methylene blue. The porous β -Bi₂O₃ nanoplates annealed for 7 h showed the best photocatalytic activity. To confirm the nanoplate photocatalyst cytotoxicity, cell viability tests were performed by treating HEK293 normal kidney cells with the porous β -Bi₂O₃ nanoplates. The porous β -Bi₂O₃ nanoplates are also characterized as negative electrode materials for supercapacitor application by cyclic voltammetry (CV) and galvanostatic charge/discharge measurements. Due to the unique architecture, the porous β -Bi₂O₃ nanoplates exhibit a high capacitance of 1685 F g⁻¹, as well as good cycling stability.

Poster Presentation : **MAT.P-376**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Characteristics of CO₂ Capture by Amine-impregnated Two-types Mesoporous Silica Spheres

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In this study, we synthesized two types of mesoporous silica materials for use as supports to amine-impregnated for CO₂ capture. One was mesoporous silica sphere (MSS) materials and the other was mesoporous hollow silica materials (MHSS). MHSS and MSS were synthesized and modified by wet impregnation with tetraethylenepentamine (TEPA) as solid adsorbents. MHSS materials were synthesized from core-shell structured polystyrene(PS) core with mesoporous silica shell. The prepared solid adsorbents were characterized by TEM, XRD, N₂ adsorption/desorption, FT-IR, and TGA and their CO₂ capture capacity was tested. The CO₂ capture performance of the adsorbent was evaluated by the gap in the CO₂ concentration of the influent and effluent gas streams at atmospheric pressure. We investigated the influence of the loaded TEPA amount on the CO₂ capture performance. An increase in the amount of loaded TEPA, improved the CO₂ adsorption capacity of the prepared adsorbents. In addition, we compared the CO₂ capture performance with the use of two types of silica materials as supports. Due to the excellent structural properties of the MHSS, MHSS is better than MSS as amine support.

Poster Presentation : **MAT.P-377**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Enhancing the Performance and Stability of Solar Cells by Applying Multifunctional Pt(II) complexes

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Photovoltaic devices have been extensively studied because of the sustainability of sunlight. Up to now, the most developed and commercialized types of photovoltaics are inorganic solar cells based on Si and GaAs. Although they achieved power conversion efficiency (PCE) above 25%, typically they cannot effectively utilize the high-energy region light (< 500 nm) due to the severe surface recombination.¹⁻² On the other hand, organic or organic-inorganic hybrid solar cells, which are promising photovoltaics with various advantages, have been struggling with the low stability of especially UV-light, heat, and humidity. Here, we present stable Pt(II) complexes with high emission quantum efficiency and easily tunable ligands. We have designed and synthesized four kinds of Pt(II) complexes and applied them as photon down-shifting layers and protect layers from surroundings for both organic and inorganic solar cells. The optical properties and solubility of these compounds were successfully adjusted by ligand tuning. The thin layers of the complexes were fabricated by using the ultrasonic spray deposition (USD) method to reduce the aggregation. With these additional layers, various types of solar cells showed the enhanced performance and stability. References Tsai, M.-L.; Tu, W.-C.; Tang, L.; Wei, T.-C.; Wei, W.-R.; Lau, S. P.; Chen, L.-J.; He, J.-H. *Nano Lett.* 2016, 16, 1, 309-313 Lopez-Delgado, R.; Zhou, Y.; Zazueta-Raynaud, A.; Zhao, H.; Pelayo, J. E.; Vomeiro, A.; Alvarez-Ramos, M. E.; Rosei, F.; Ayon, A. *Sci. Rep.* 2017, 7, 14104

Poster Presentation : **MAT.P-378**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Optical Humidity Sensor of Randomly-distributed polydisperse Titania Particles

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Jerome Hyun***

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Measuring the relative humidity is important in a wide range of industries including agricultural, pharmaceutical, chemical, and health care. To this end, various humidity sensors, using optical, gravimetric, capacitive, and resistive mechanisms, have been proposed and used for moisture measurement. In this work, we designed a simple optical humidity sensor, expressing structural color change under different relative humidities. Our humidity sensors employ structural colors from disordered arrays of TiO₂ microspheres, which allows the sensors to be fabricated using a scalable and cheap hydrothermal method. We have previously shown examples of such structural colors from randomly-distributed polydisperse anatase TiO₂ microspheres [1]. The display of color from such an arrangement is due to the fact that the noisy ‘white’ scattering spectra from individual particles can be weight-averaged according to the particle size distribution, yielding smooth variations in the overall scattering and extinction spectrum in the visible range. In this work, we show through the synthesis of amorphous, porous titania microspheres, reversible modulation of the ensemble scattering properties between dry and humid conditions. In humid conditions, water vapour diffuses into the dense porous sites within the particles and condenses within the pores, altering the overall refractive index, thereby changing the scattering properties. The use of disordered medium further enables the sensors to provide important physiochemical information such as the porosity and enthalpy of adsorption, using a fraction of material required by traditional gravimetric techniques.[1] Alam, A-M; Baek K; Son J; Pei Y-R; Kim D-H; Choy J-H; and Hyun J-K., ACS Appl. Mater. Interfaces, 2017, 9 (28), 23941– 23948

Poster Presentation : **MAT.P-379**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Characterization of ZnO@SiO₂ Nanocomposites Grown on Halloysite Nanotubes for Adsorption of Organic Dyes

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Halloysite nanotubes (HNTs) are an aluminosilicate clay with the kaolin group ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 \cdot 2\text{H}_2\text{O}$). The outer surface of the HNTs comprises a silicate negative charge layer, whereas the inner surface comprises an alumina positive charge layer. With this feature, HNTs have adsorption ability of dye molecules. In this study, to enhance the adsorption ability of HNTs, we synthesized ZnO@SiO₂ nanocomposites grown on halloysite nanotubes. We compared the adsorption ability of this synthesized HNTs-ZnO@SiO₂ and HNTs for a kind of dye, methylene blue (MB) existed in textile, paper, printing and other industrial wastewater. MB has a positive-charged functional group. Therefore, we expect that MB can be effectively adsorbed on newly synthesized HNTs-ZnO@SiO₂ and HNTs. The adsorption ability of HNTs-ZnO@SiO₂ and HNTs for MB were examined by ultraviolet-visible spectroscopy and the surface charge of HNTs-ZnO@SiO₂ and HNTs was measured by zeta potential. It was found that the adsorption ability of HNTs-ZnO@SiO₂ nanocomposites for MB was largely increased because they have higher negative surface charge compared with HNTs

Poster Presentation : **MAT.P-380**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

SnO₂ Nanowire Gas Sensors Decorated with V₂O₅ Nanoisland for Selective NO₂ Sensing

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SnO₂ nanowires decorated with V₂O₅ nanoisland were prepared by atomic layer deposition (ALD) and investigated as sensing layer. For the V₂O₅ to be coated on the SnO₂ nanowires in a nanoisland form, thin VO_x amorphous layers were initially deposited on the SnO₂ nanowires via ALD, and then annealed at various temperatures. Morphological analysis based on transparent electron microscopy indicate that the V₂O₅ layers appear to agglomerate during the anneal process, leading to nanoisland formation on the surface of SnO₂ nanowires. In gas sensing experiment, the annealed nanoisland heterostructures exhibit more enhanced gas response and selectivity toward NO₂ target gas compared to the V₂O₅ /SnO₂ core-shell structure, where the nanotube is completely covered with V₂O₅ layer. Based on our density functional theory calculation, SnO₂ is more favorable to absorption of NO₂ gas than V₂O₅, indicating the partial decoration of V₂O₅ nanoisland plays an important role in improving the sensing performance. Corresponding author*Email: immrc@kitech.re.kr

Poster Presentation : **MAT.P-381**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Ag₂O/Fe₂O₃ Heterostructures Encapsulated with Reduced Graphene Oxide for Improving Photocatalytic Performance

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Reduced graphene oxide has attracted a great deal of attention in many of the scientific and engineering fields owing to its fascinating physicochemical properties, such as electronic conductivity, large surface area, and superior chemical stability. Furthermore, an excellent electron capturing ability allows the reduced graphene oxide to couple with semiconductor photocatalysts for improving photocatalytic efficiency. Herein, we present Ag₂O/Fe₂O₃ heterostructures that are encapsulated with the reduced graphene oxide. In these structures, the Ag₂O/Fe₂O₃ composites where the Ag₂O nanoparticles are uniformly coated onto surfaces of the flower-like Fe₂O₃ microspheres appear to be densely anchored on the reduced graphene nanosheets. The graphene-based heterostructures exhibit more enhanced visible-light driven photocatalytic performance in the removal of organic pollutant compared with the bare heterostructures without the reduced graphene oxide matrix. Moreover, they were proven to be more efficient in the water splitting experiment. The improved photocatalytic performance can be assigned to the increased surface area, fast charge separation and thus suppressed recombination of photogenerated electron-hole pairs by adopting the reduced graphene oxide as a photocatalytic matrix. Corresponding author*Email: immrc@kitech.re.kr

Poster Presentation : **MAT.P-382**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Highly Luminescent Octahedral Rhenium Metal Cluster with Large Stokes shift and Application to Transparent Luminescent Solar Concentrators

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The LSC is a device that employs luminescent dyes to concentrate the sunlight on PVs (Si cells) attached through the polymer waveguide. It has many advantages such as the possibility of various designs with very high transparency and desirable shape and color. It is also economically competitive and can be processed in the air. We applied octahedral rhenium clusters as a luminophore, which has transparency due to the low absorption at visible range and zero-reabsorption due to the massive Stokes shift. The metal clusters, $(\text{Bu}_4\text{N})_4[\text{Re}_6\text{S}_8(\text{NCS})_6]$, prepared by reaction of $(\text{Bu}_4\text{N})_4[\text{Re}_6\text{S}_8\text{Cl}_6]$ with molten KSCN were uniformly mixed with PMMA. The LSC with octahedral rhenium cluster exhibit >90% transparency and >1.5% efficiency depending on various concentrations.

Poster Presentation : **MAT.P-383**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation and characterization of CuO/ TiO₂ composite hollow spheres with excellent photocatalytic performance under visible light irradiation

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TiO₂ was one of the most important n-type semiconductors and has been recognized as a promising photocatalyst for degradation of organic compounds. Moreover, because of hollow structured TiO₂ has higher specific surface area, lower density, better permeation, an greater light harvesting capacity, it exhibits superior photocatalytic activity over conventional particle materials. However, TiO₂ can only be excited for photocatalytic reaction under UV light because of its wide bandgap(~3.0or3.2eV). To over come these draw backs, numerous efforts have been made to modify the surface of TiO₂, or combine TiO₂ with metal,non-metal, and organic molecules. It is expected that enhanced visible light photocatalyti cactivity could be achieved using the modified TiO₂ as photocatalysts. In this study, we synthesized CuO/TiO₂ composite hollownanospheres(CuO/TiO₂HS) using polystyrene as a template. The average diameter, shell thickness, crystalline structure, and composition of CuO/TiO₂HS were characterized by using Transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The optical absorption property of the CuO/TiO₂HS was measured by using UV-Vis absorption spectrum. The photocatalytic activity of the samples was characterized by degrading 10 mg·L⁻¹methyleneblue under visible light irradiation. As a result, CuO/TiO₂HS exhibited better photocatalytic activity than the pure TiO₂ nanoparticles and TiO₂ hollow nanospheres. The improvement in photocatalytic activity was caused by the enhanced light absorption in the visible light region.

Poster Presentation : **MAT.P-384**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

SnO₂ nanotube gas sensors synthesized by template-assisted atomic layer deposition

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SnO₂ nanotube gas sensors were synthesized by template-assisted atomic layer deposition (ALD). For the first step to grow the SnO₂ nanotube, we prepared VLS-grown TeO₂ (Tellurium oxide) nanowires as inorganic templates. An amorphous SnO_x layer is then deposited on the TeO₂ nanowire by ALD, and annealed at various temperatures from 700 to 900°C. The XRD results revealed that polycrystalline SnO₂ was successfully synthesized with tetragonal structure. SEM and TEM images show that the prepared SnO₂ nanotubes have a 1-dimensional structure with a length of few-micro meters and diameter of ~120 nm, and the crystal size of SnO₂ nanotubes varies with annealing temperatures. In gas sensing experiment, the SnO₂ nanotube exhibit more enhanced gas response toward NO₂ target gas with fast response/ recovery behavior as the annealing temperature increases. The improved sensing properties can be attributed the reduced grain size of SnO₂ nanotubes, and thus increasing surface area upon high temperature anneal. Corresponding author*Email: immrc@kitech.re.kr

Poster Presentation : **MAT.P-385**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Cr-doping reinforce lattice stability of low temperature phase of VO₂

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We have prepared Cr-doped VO₂ film (Cr_xV_{1-x}O₂) on c-cut sapphire plate (0001). The VO₂ lattice could accommodate the impurity level up to, but the metal to insulator transition (MIT) of VO₂ behavior observed only on resistance and transmittance measurements in the temperature range of 290 – 380 K. The starting point of metal to insulator (T_{CS}) keep nearly 350 K, but the starting point of insulator to metal transition (T_{HS}) shifted from 308 K to 320 K. In the high doping level of Cr, the T_{CS} also shifted from 350 K to 370 K. This indicates the Cr-doped VO₂ lattice especially stabilized at the low temperature region, below the metal to insulator temperature (T_C) of the VO₂. The gap between T_{HS} and T_{CS}, which the intermediated region (percolation conduction region) between metal and insulator, narrowed by the doping. This observed doping effect is reversed behavior which observed in W-doped VO₂.

Poster Presentation : **MAT.P-386**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Sensor applications of graphitized carbon nanotubes decorated with gold nanoparticles by conversion of sucrose using AAO template

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This work describes a simple fabrication of gold nanoparticles (AuNPs) attached carbon nanotubes (AuCNTs) and their applications as field effect transistor (FET) sensor. The preparation of AuCNTs was performed through the carbonization of sucrose based on anodic aluminum oxide (AAO) template. The AAO template with ordered channel decorated with AuNPs was fabricated by a thermal decomposition of HAuCl₄. The size of high crystalline AuNPs attached to AAO template have ~20 nm diameter. The crystallinity of the graphitized carbon phase was confirmed by analyzing the G and D bands in their Raman spectra. The fabricated AuCNTs, which a neat and straight tube, will be applied as FET sensor for carbohydrates detection and compared with our previous AuNPs-MWCNT FET sensor showing the high sensitivity.

Poster Presentation : **MAT.P-387**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Light-induced Multi-switch via Photo-responsive Polymer/Quantum Dot Nanocomposites

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Light is an attractive source as a stimulus since it can precisely control both temporally and spatially by changing the wavelength and intensity without any physical contact. Therefore, photo-responsive materials such as photo-switchable molecules and quantum dots are actively studied. Azobenzene, a representative photo-switchable molecule, incorporated material changes its structure whereas perovskite quantum dots can emit light of a specific wavelength upon irradiation.[1,2] Herein, we have developed a multi-switch material which can be controlled by different wavelengths of light by synthesizing a composite of photo-responsive polymer and quantum dots. Photo-responsive polymer can be synthesized by azobenzene-functionalized polydimethylsiloxane, and perovskite quantum dots can be embedded in the polymer by previously reported method. The structural change and luminescence of photo-responsive nanocomposite material can be simultaneously controlled. As a result, we suggest four-states multi-switch by changing wavelength of the applied light which can concurrently control the photo-deformation and photoluminescence (PL): (i) light OFF & bending ($\lambda > 503$ nm), (ii) light ON & bending ($\lambda > 365$ nm), (iii) light OFF & stretched ($\lambda = 365$ nm), and (iv) light ON & bending ($\lambda < 365$ nm). We anticipate our approach can be not only applied to various flexible and transparent optical devices, but also transfer information as logic gates (00₍₂₎, 01₍₂₎, 10₍₂₎, 11₍₂₎). References 1.W. Cha, H. Kim, S. Lee and J. Kim, J. Mater. Chem. C 5, 6667 (2017). 2.W. Lee, D. Kim, J. Lim, G. Kim, I. Kim, S. Kim, J. Kim, Sensors and Actuators B: Chemical, 266: 724-729 (2018).

Poster Presentation : **MAT.P-388**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Printing of interdigitated electrodes pattern for 2nd generation open paper based DMF chip

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Paper is cheaper and more flexible than conventional materials like wafer and can be easily used and discarded. Currently, our lab is studying how to use paper in various fields including lab-on-a-chip technology. In addition, for various experiments using paper, various printing techniques including inkjet printing are utilized. In paper-based DMF chip using Electrowetting on dielectric layer, all droplet manipulations are effective only when fluids are operated between two dielectric layers with channel gaps less than 300 μm to reduce the surface tension. As a result, the liquid volumes are confined to several microliters at most. Moreover, EWOD only works with polar molecules like water and has weak force. To solve these issues, dielectrowetting is applied to achieve creating, transporting, splitting and merging of droplets in open space and with non-polar molecules. If the applied electric field is uniformed, the magnitudes of the electrostatic forces applied on the upper and lower sides of the polarized particles are identical to each other, so the net force applied on the particles becomes zero and the particles do not move. However, when the electric field applied on the particles is not uniformed, the magnitude of the electrostatic forces applied on the particles are different from each other, then the particles are translocated to the dense part of electric field due to the gradient of the electric field. Therefore, in the interdigitated electrodes, due to difference of electric field density, liquid dielectrophoresis occurs. References[1] Hongyao Geng, Jian Feng, Lisa Marie Stabryl and Sung Kwon Cho, Lab Chip, 2017, 17, 1060[2] A.M.J. Edwards, C.V. Brown, M.I. Newton, G. McHale, Current Opinion in Colloid & Interface Science 36 (2018) 28–36

Poster Presentation : **MAT.P-389**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

ZnIn₂S₄, synthesized by solvothermal method, mixed with ordered mesoporous carbon for anode material of LIB

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Lithium ion batteries (LIB) are efficacious electrochemical energy storage device due to their high energy density, long life cycle, and no memory effect. Graphite is the most commonly used anode for LIB because of its stability and low volume expansion. However, graphite has critical disadvantage, low theoretical capacity. To overcome this limitation, the development of high-capacity anode material is indispensable. Layered ternary chalcogenide system, Zinc Indium Sulfide (ZnIn₂S₄) exhibits two polymorphs based on cubic and hexagonal lattices. When zinc indium sulfide with hexagonal lattices act as an anode material in lithium ion battery, it shows interesting features. In₂S₃ has layered structure with proven high theoretical capacity and ZnS has reversible lithium insertion/desertion with good stability. From these features, ZnIn₂S₄ could be a good anode material for LIB. Also, carbon-based materials have been widely introduced due to its excellent conductivity. On the other hand, ordered mesoporous carbons are good candidates for heterogeneous energy storage composites due to its regular structure and large surface area which could facilitate higher material utilization for electrochemical redox reactions. Zinc indium sulfide will be mixed with ordered mesoporous carbon and show enhanced electrical conductivity. In this work, ZnIn₂S₄/C nanocomposites are synthesized with CMK-3 and tested for anode material in lithium ion battery. Characterization methods are X-ray diffraction, Nitrogen sorption, SEM, and various electrochemical investigations. We anticipate that these materials may show good cycle ability, stability, and high rate performance.

Poster Presentation : **MAT.P-390**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Development of NanoSensors Based on Silica Nanotube Capped with Enzyme Substrates Triggered by Enzymatic Degradation.

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Silica nanotube (SNT) can store and transport nanomaterials such as organic molecules, nanoparticles, genes and drugs as a nano-sized carrier. It was revealed that protease assay based on preparation of target specific capped SNTs system has a reliable sensitivity and selectivity. Gourd SNTs (GSNTs) were fabricated by using Ar plasma treatment. Then partial modification at open ends of the GSNTs was done by using Al₂O₃ microbead. And specific amino acids and alkyl chain linkers mediated sequences were immobilized near the open ends of GSNTs to build a cap. The capped GSNTs (CGSNTs) were tested their efficiency by fluorescence measurement. Detection limit based on CGSNT template by acquiring the fluorescence signal was less than 1 ng. And IC₅₀ was determined by inhibitor under the CGSNT based template system. The CGSNT template can be applied a versatile platform for protease assay or bioapplication due to its reliable sensitivity, selectivity and simple handling.

Poster Presentation : **MAT.P-391**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

NMR based analysis about two dimensional structure of graphitic carbon nitride for labeling ^{13}C -, ^{15}N - and their Hydrogen-bonding at oligomer.

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Graphitic carbon nitride (g-C₃N₄) is attention as eco-friendly photocatalyst and bio-imaging. g-C₃N₄ has a three dimensional structure via polymerization of melamine and melem unit. recent studies seek to establish an alternative synthetic approach for two-dimensional g-C₃N₄ using a smaller precursor such as urea. However, the effectiveness of such a synthetic approach and resultant polymeric forms of g-C₃N₄ in this approach are still largely unknown. In this study, we present that solid-state NMR (SSNMR) analysis for ¹³C- and ¹⁵N-labeled g-C₃N₄ prepared from urea offers an unparalleled structural view for the heterogeneous in-plane structure of g-C₃N₄ and most likely for its moieties. We revealed that urea was successfully assembled in melem oligomers, which include extended oligomers involving six or more melem subunits. SSNMR, transmission electron micrograph, and ab initio calculation data suggested that the melem oligomer units were further extended into graphene-like layered materials via widespread NH–N hydrogen bonds between oligomers.

Poster Presentation : **MAT.P-392**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Single anion open framework structured KFeO_2 as high energy density cathode for potassium ion batteries

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Potassium ion batteries (KIBs) is emerging as a promising energy storage technology due to low cost and high energy density relative to sodium ion battery. However, reversible electrochemical (de)insertion into host structure is hindered by the large size of K^+ ion that limits the choice of suitable electrode materials for KIB. KFeO_2 was found to crystalized in orthorhombic crystal structure with Fe^{3+} ion stabilized in tetrahedral site. Here, for the first time we have examined the electroactivity of $\text{Fe}^{3+/4+}$ in open framework type KFeO_2 . The cathode material delivered 55 mAh/g discharge capacity at 10mA/g current density when charged to 3.9V (vs. K/K^+). Structural and chemical composition of the charged electrode was subjected to ex-situ XRD, EDX and XPS analysis

Poster Presentation : **MAT.P-393**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Electrochemical characterization of KFeSO_4F with a KTiOPO_4 structure type

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Recently, a number of studies are being progressed to discover the high performance cathode material in potassium ion batteries (KIBs). Potassium has a low standard reduction potential that is almost same as lithium (-2.93 vs. -3.04 V), which implies the possibility that high-voltage full-cells can be constructed without a loss of significant energy densities. KFeSO_4F (KFSF) is an active polyanionic material, which is isostructural to $\text{KTiO}(\text{PO}_4)$ (KTP). A KTP structure has a 3-D diffusion channel. $\text{KV}(\text{PO}_4)\text{F}$ and $\text{KVO}(\text{PO}_4)$ are also synthesized with a KTP type and their electrochemistry has been already studied. Orthorhombic KFSF, high-temperature phase, was studied by Tarascon group and was revealed to be electrochemically active for K^+ -extraction/insertion. The electrochemical performance of a low-temperature phase KFSF (monoclinic) was not comparable to that of orthorhombic KFSF. Though orthorhombic KFSF was expected to be attractive as a KIB cathode, however, they did not provide comprehensive electrochemical results. In the present study, we will show the synthetic process of orthorhombic KFSF and structure identification by XRD patterns. Electrochemical characterization of KFSF by various analytical methods including cyclic voltammetry and charge/discharge curve will be also described to show that KFSF could be a viable cathode in KIBs.

Poster Presentation : **MAT.P-394**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

KCrS₂ Cathode with Considerable Cyclability and High-rate Performance: The First K⁺-Stoichiometric Layered Compound for Potassium-Ion Batteries

Anthonisamy nirmalesh Naveen, Myoungho Pyo*

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KCrS₂ is presented as a stable and high-rate layered-material that can be used as a cathode in potassium-ion batteries (KIBs). To the best of our knowledge, KCrS₂ is the only layered-material with stoichiometric amounts of K⁺, which enables coupling with a graphite anode for full-cell construction. Cr(III)/Cr(IV) redox in KCrS₂ is also unique, because LiCrS₂ and NaCrS₂ are known to experience S²⁻/S₂²⁻ redox. O3-KCrS₂ is first charged to P3-K_{0.39}CrS₂ and subsequently discharged to O'3-K_{0.8}CrS₂, delivering an initial discharge capacity of 71 mAh·g⁻¹. The following C/D shows excellent reversibility between O'3-K_{0.8}CrS₂ and P3-K_{0.39}CrS₂, retaining ca. 90% of the initial capacity during 1000 continuous cycles. The rate performance is also noteworthy. A C/D rate increase of 100-fold (0.05C to 5C) reduces the reversible capacity only by 39% (71 to 43 mAh·g⁻¹). The excellent cyclic-stability and high-rate performance are ascribed to the soft sulfide-framework, which can effectively buffer the stress caused by K⁺ de-insertion/insertion. During transformation between P3-K_{0.39}CrS₂ and O'3-K_{0.8}CrS₂, the material resides mostly in the P3-phase, which minimizes the abrupt dimension-change and allows facile K⁺ diffusion through spacious prismatic sites. Structural analysis and density-functional-theory calculations firmly support this reasoning.

Poster Presentation : **MAT.P-395**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

A Beneficial Role of Fullerene (C₆₀) as a Hybridization Matrix for Improving the Electrochemical Performance of Layered Double Hydroxide

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An effective way to explore high performance electrode for supercapacitor is developed by employing 0D fullerene (C₆₀) nanocluster as a hybridization matrix for 2D layered double hydroxide (LDH) nanosheets. The electrostatically-driven self-assembly of cationic LDH nanosheets with anionic C₆₀ nanoclusters yields intimately-coupled nanohybrids of the C₆₀-Ni-Fe-LDH. Of prime importance is that the C₆₀-Ni-Fe-LDH nanohybrid shows better capacitances with better cyclability than the pristine C₆₀ and Ni-Fe-LDH. Since there occurs significant electron transfer from electron-donating LDH nanosheet to electron withdrawing fullerene, the hybridization with C₆₀ results in the enhancement of the charge transfer kinetics of Ni-Fe-LDH. The present study clearly demonstrates that the hybridization with fullerene is quite effective in improving the electrode performance of LDH nanosheets.

Poster Presentation : **MAT.P-396**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Mg/Al-Layered Double Hydroxide Nanosheet Oxidants

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Nanomaterials like graphite and carbon nanotube can be intentionally oxidized for various purposes and applications. Various organics and metals are also oxidized to tune their electronic structure, modify their surface chemistry, and create new functionalities. Unfortunately, however, most oxidation methods use toxic chemicals and high energy-consumption processes, which are harmful to the environment and humans. Herein, we examined the possibility of replacing existing oxidation methods with the newly synthesized layered double hydroxide (LDH) approach.

Poster Presentation : **MAT.P-397**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Superhydrophobic Sponges with pH Tuning Ability for Pollutant Purification

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Abstract Pollutions caused by oil spill accidents and industrial discharges have been recognized as a particularly severe environmental issue. Thus, oil/water separation has been of great interest in recent years. Many efforts have been focused on the development of advanced techniques and materials for effective oil/water separation. However, most such techniques and materials are able to separate oil or water layer only. They also suffer from the limitation of high fabrication cost due to multisteps and complex process. Thus, a simple process technique to solve or address abovementioned issues is urgently required for simultaneous separation of oil as well as water layers. We report novel one step technique to fabricate superhydrophobic sponge capable of separating oil as well as water. References[1] N. R. Han, Y. T. Lim, W. R. Jang, H. Y. Koo, W. S. Choi Polydopamine-mediated all-in-one device with superhydrophilicity and superhydrophobicity for one-step oil/water separation and pollutant purification. *Polymer* 107, 2016, 1-11.[2] Y. T. Lim, N. R. Han, W. R. Jang, W. Y. Jung, S. W. Han, H. Y. Koo, W. S. Choi Surface Design of Separators for Oil/Water Separation with High Separation Capacity and Mechanical Stability. *Langmuir* 33, 2017, 8012-8022.

Poster Presentation : **MAT.P-398**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

An Effective Way to Improve the Electrocatalytic and Li-O₂ Electrode Functionalities of α -MnO₂ Nanowire via Tuning of Chemical Bonding Nature

Tae-Ha Gu, Xiaoyan Jin, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The surface anchoring of highly oxidized selenate (SeO_4^{2-}) cluster is exploited as a novel strategy to synthesize efficient MnO₂-based oxygen electrocatalyst and Li-O₂ electrode. The bond competition between neighboring (Se^{6+} -O) and (Mn-O) bonds is quite effective in stabilizing Jahn-Teller-active Mn³⁺ state and in increasing oxygen electron density of α -MnO₂ nanowire. The selenate-anchored α -MnO₂ nanowire shows excellent oxygen electrocatalytic activity and electrode performance for Li-O₂ batteries, which is due to the improved charge transfer kinetics and reversible formation/decomposition of Li₂O₂. The present study underscores that the anchoring of highly oxidized cluster anion can provide quite efficient way of improving the electrocatalytic performance and electrochemical performances of nanostructured metal oxide in Li-O₂ cells.

Poster Presentation : **MAT.P-399**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Optimization of the Stacking Structure and Electrochemical Functionalities of Co-Al-Layered Double Hydroxide Nanosheets

Najin Kim, Tae-Ha Gu, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

An effective chemical way to optimize the electrochemical functionalities of layered double hydroxide (LDH) is developed by the controlled restacking of exfoliated 2D nanosheets. The fine-control of the stacking number and pore structure of restacked Co-Al-LDH nanosheets with positive layer charge can be achieved by changing the hydration radius and charge density of intercalant anion. As the hydration radius increases, charge density of intercalant ion decreases and the stacking number of LDH nanosheets becomes smaller. Due to the resulting expansion of surface area and the shortening of ion diffusion path, a decrease of the stacking number of restacked Co-Al-LDH nanosheet is quite effective in improving its electrode performance for supercapacitor. Also, the controlled restacking of Co-Al-LDH nanosheet enhances its electrocatalytic performance for oxygen evolution reaction. The present study clearly demonstrates that the controlled restacking of exfoliated LDH nanosheets with various anions can provide an effective way to optimize the electrode and electrocatalyst functionalities of LDH materials.

Poster Presentation : **MAT.P-400**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

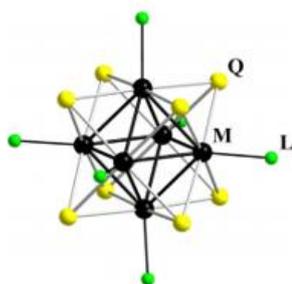
Synthesis and structure of rhenium clusters as new candidates for solar cell application.

Thi giang Ly, Sung-Jin Kim^{1,*}

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

¹*Department of Chemistry, Ewha Womans University, Korea*

In recent years, there has been increasing interest in photoluminescent octahedral clusters [$\{M_6Q_8\}L_6$] (where M is Mo, W or Re; Q – inner ligands) materials. In particular, hexanuclear rhenium(III) cluster complexes with wide variety of chemical and physical properties are the most potential candidate among the family of rhenium cluster compounds. Because of excellent photoluminescent properties, octahedral rhenium clusters are significant materials for various applications, such as solar cell, light emitting and biological application. In the present study, the new cluster $[Re_6Q_8(TBP)_5(SO_3)]$ (where Q is Se or S) was synthesized and characterized. The structures were confirmed by chemical analysis and energy-dispersive X-ray spectroscopy methods.



Octahedral rhenium cluster core



$Na_{10}[Re_6Se_8(SO_3)_6]$

$Na_{10}[Re_6S_8(SO_3)_6]$

Poster Presentation : **MAT.P-401**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

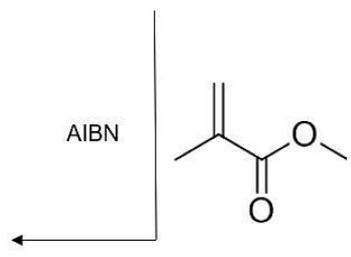
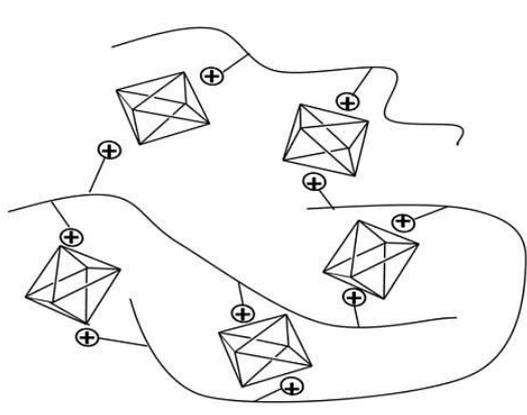
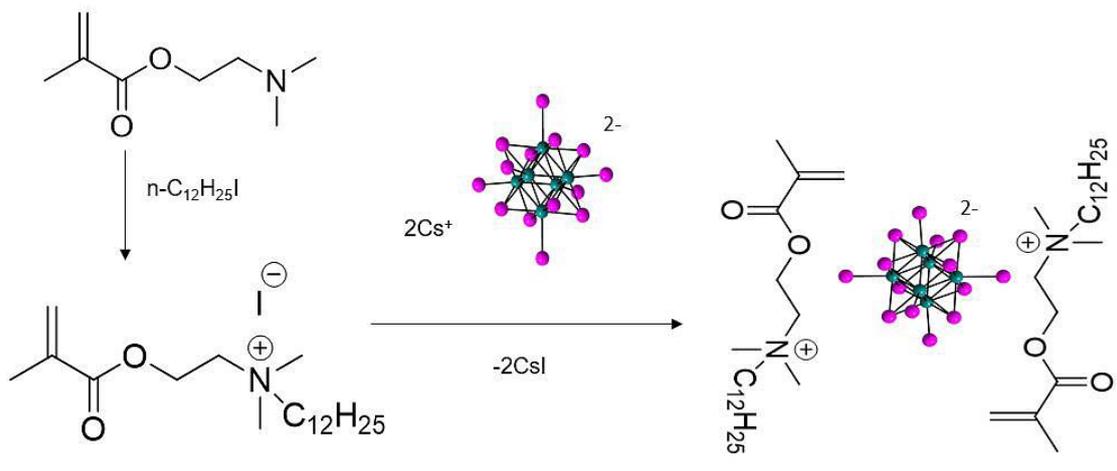
Highly Emissive Octahedral Molybdenum Metal Cluster-Polymer Hybrid and Application on Large Window

Dieu Nguyen, Sung-Jin Kim^{1,*}

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

¹Department of Chemistry, Ewha Womans University, Korea

A new luminescent, highly efficient solar concentrator (LSC) that consisted of nanosized metal-clusters as molecular luminophores encapsulated in poly(methyl methacrylate) (PMMA) waveguide is fabricated by simple solution process. To make a highly emissive, transparent, and robust LSC, organic-inorganic salts such as (dMDAEMA)₂[Mo₆I₁₄] (where dMDAEMA⁺ refers organic cation, 2-(methacryloyloxy) ethyl dimethyldodecylammonium) are uniformly incorporated in PMMA. Due to the strong absorption at UV-Vis wavelength up to (~500 nm) and the large Stokes shift to the near infrared (~850 nm) emission, this hybrid luminophore allows zero reabsorption resulting efficient UV-Vis sunlight harvesting with low tint. Si photovoltaic cell with dimensions of 2.0 x 0.3 cm² is placed at the edge of the LSC plate with dimensions of 2.0 x 2.0 x 0.3 cm³. The highest power conversion efficiency (PCE) 1.74% and transparency ~90% observed in this LSC system are significantly higher than previous known LSC systems. In addition to the high power conversion efficiency, its chemical robustness and simple solution process in fabrication suggest a promising future direction for the development of a practical LSC system for a transparent building-integrated energy harvesting smart windows.



Poster Presentation : **MAT.P-402**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Solution process of P, N co-doped graphene-based as efficient metal-free electrocatalyst for oxygen reduction reaction

Dawoon Jang, Sungjin Park*

Department of Chemistry, Inha University, Korea

Graphene-based materials are promising as metal-free, cost-effective electrocatalysts owing to their feasibility for mass production and excellent electrochemical properties. Recently, heteroatom co-doping of graphene networks has been identified as a promising route to produce efficient electrocatalysts for the oxygen reduction reaction (ORR). However, generally N doped carbon based materials have been heat treated at high temperatures to increase ORR performance. In this study, we have synthesized a P, N co-doped graphene-based material (N-P-rG-O) using a two-step solution process in which graphene oxide is sequentially reacted with phytic acid and ammonium hydroxide in water. The N-P-rG-O catalyst exhibits an onset potential for the ORR in basic medium (0.1 M KOH) of 0.89 V (vs. the reversible hydrogen electrode), following a four-electron pathway and showing excellent stability against methanol poisoning in durability tests.

Poster Presentation : **MAT.P-403**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

3D steam-activated graphene/CNT hybrid frameworks for improving cyclic capacities to store lithium ions

Yunseok Shin, Sungjin Park*

Department of Chemistry, Inha University, Korea

Carbon-based materials are considered as a promising active or supporting material for the lithium ion batteries (LIBs). Especially, assembly of two-dimensional (2D) graphene into the three-dimensional (3D) internetworked architecture is of crucial importance because it combines the intrinsic physical properties. Herein, we demonstrate the unique hierarchical structures, where carbon nanotubes (CNTs) are branched onto the modified surfaces of 3D, steam-activated reduced graphene oxide (sRG-O) frameworks, prepared by self-assembly, steam activation, and microwave methods. The surface sites of 3D sRG-O are critical for controlling crystalline structure and deposition density of Fe₃O₄ nanoparticles through a microwave induced synthesis, as well as for providing a large surface area and conducting pathway. Simultaneously, the bamboo-like CNT branches are grown on the Fe₃O₄ nanoparticles acting as catalysts to stabilize and conductively connect 3D sRG-O/Fe interparticles for the enhanced rate and cyclic performances of LIB.

Poster Presentation : **MAT.P-404**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Pomegranate-like Bulk Adsorbents for Removal of Heavy Metal Ions

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Heavy metal ion discharges from industrial processes have become a serious environmental problem because of their high bioaccumulation characteristics. Thus, the removal of heavy metal ions is important for human beings and the environment. Nano/micro-adsorbents show a high specific surface area relative to the volume, which enables nano/micro-adsorbents to be a potential candidate for adsorbent with a high performance. However, it has been recently reported that the unintended leakage of nano/micro-materials into the environment can cause a significant threat to the environment and public health. To address this problem, we developed a bulk adsorbent containing three types of nano/micro-adsorbents for removal of heavy metal ions.

Poster Presentation : **MAT.P-405**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis of Sponge Typed Air Filters for Removal of PM

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Department of Chemical & Biological Engineering, Hanbat National University, Korea

Removal of particulate matter (PM) has attracted worldwide attention due to the increase of air pollution caused by rapid industrialization and urbanization. The PM is mainly emitted by artificial sources such as activity of industries and combustion of fuels. The PM, also known as particle pollution, is a complex mixture of extremely small particles and liquid droplets that get into the air. Once inhaled, these particles can affect the heart/lungs and cause serious health effects. The PM is classified as first-class carcinogens by the WHO. Thus, many efforts have been focused on the developing noble techniques to effectively remove or filter the PM. We developed specially designed filters with a high performance for removal of PM10 and PM2.5.

Poster Presentation : **MAT.P-406**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

An anti-overturn Janus sponge with excellent floating stability for simultaneous pollutant remediation and oil/water separation

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Department of Chemical & Biological Engineering, Hanbat National University, Korea

Harsh marine conditions such as high waves and winds prevent effective oil/water separation and reduce the level of separation performance that is obtained in the laboratory. For real applications of marine pollution remediation, an anti-overturn Janus sponge (AJS) that partially floats/is partially submerged on/under water was prepared. The Janus characteristic originates from the cooperative effect of the hydrophilic part absorbing water and the hydrophobic part generating buoyancy. The AJS with an appropriate hydrophilic/hydrophobic ratio showed excellent floating stability under high waves and strong winds. The AJS also exhibited high adsorption of aqueous pollutants during fast oil/water separation due to its Janus characteristic, stably remained at the oil/water and water/oil interfaces in three liquid multiphases and removed aqueous pollutants at each interface. Because of its great control over the alteration of the ratio, structure, and shape of its hydrophilic and hydrophobic parts, the AJS can be transformed into various types of structures on demand. A pant-like structure that was divided into two branches could successively separate three liquid multiphases (light oil/water/heavy oil) and quickly purify contaminated water during the separation.

Poster Presentation : **MAT.P-407**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Effect of synthetic conditions on material structure and photocatalytic performance of carbon nitride synthesized from different precursors

Sujin Seok, Sungjin Park*

Department of Chemistry, Inha University, Korea

Graphitic carbon nitride (g-C₃N₄)-based materials show excellent performance as photocatalysts because of their band gap of ~2.7 eV allowing visible light harvesting, high population of N-associated sites, and porous structure. In particular, g-C₃N₄-based materials are highly attractive metal-free photocatalysts for the visible-light-induced degradation of organic pollutants. The photocatalytic degradation of organic pollutants such as rhodamine B (RhB) is of great industrial and environmental importance. Herein, we study the relation between materials' structures and photocatalytic properties for RhB degradation depending precursors (dicyandiamide, melamine, and urea) and synthetic conditions (direct heating and sequential heating). We found that the most efficient g-C₃N₄-based photocatalysts for organic pollutant degradation could be prepared by sequential heating of urea as a precursor probably due to their larger surface areas.

Poster Presentation : **MAT.P-408**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Intercalating Conjugated Polyelectrolytes (CPEs) into Layered Titanium dioxide sheets for Improving Photocatalytic Effect

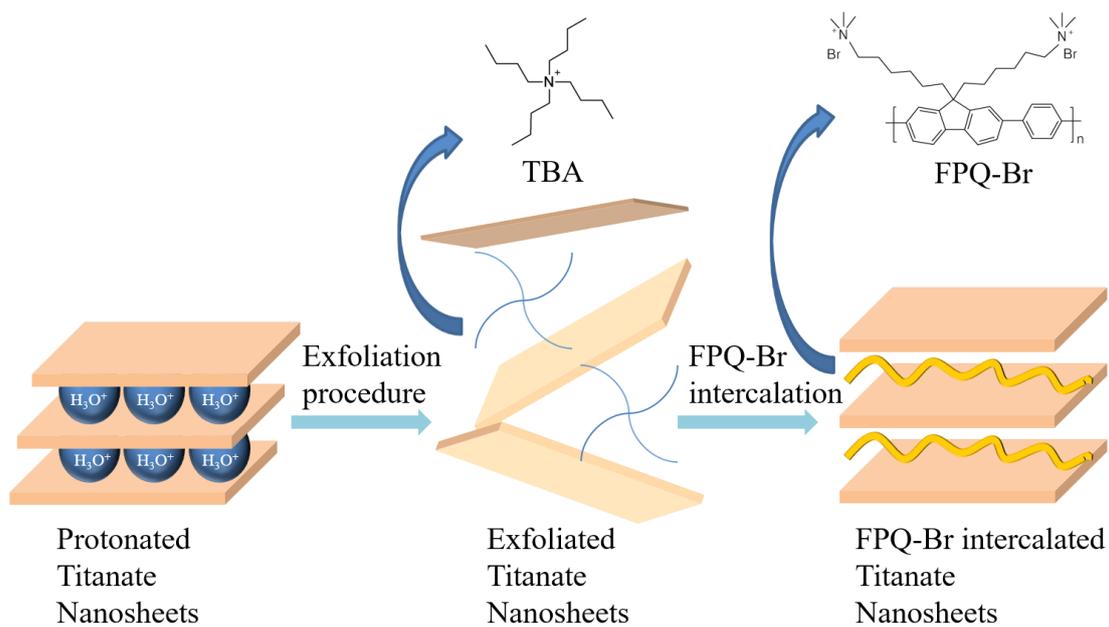
Seongwon Hong, Jin Kuen Park^{1,*}

Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Cationic π -conjugated polyelectrolytes (CPEs) were successfully intercalated into layered titanate (TiO₂), while exfoliated layered titanates were reassembled into lamellar structures. The resulting composites showed significantly enhanced visible light absorbance and enhanced photocatalytic activity with respect to layered titanate, which was proven by the photodegradation of methylene blue in aqueous media under irradiation by visible light. Notably, some amount of tetrabutylammonium (TBA) used for the delamination of a layered titanate could be co-intercalated with CPEs, and the residual TBA could be removed via continuously repeating the intercalation process, maintaining the spatial arrangement and content of CPEs in the confined area of layered titanates. However, with the presence of TBA, the hybrid demonstrated greater performance in the photodegradation of methylene blue at any given period of time and almost complete degradation of such dye within 4 minutes. The significant difference in photocatalytic efficiency with or without TBA suggested that the TBA effectively reduced the surface energy at the interface between the organic components and aqueous medium, which was evidenced by the dispersity assessment of hybrids with or without TBA.

Scheme 1. Two steps for fabricating FPQ-Br intercalated layered titanate nanosheets



Poster Presentation : **MAT.P-409**

Material Chemistry

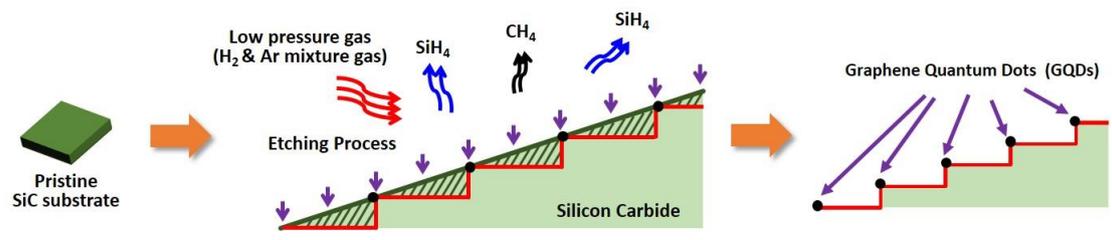
Grand Ballroom, THU 11:00~12:30

Biocompatible Graphene Quantum Dots by Thermal Decomposition of Silicon Carbide without the use of chemicals

Naeun Lee

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Korea*

Graphene quantum dots (GQDs) are expected to be used in bio-fields due to unique optical properties and low toxicity. However, complicated process and poor quality of GQDs at still issues to be solved. We reported a fabrication of high quality GQDs by thermal decomposition of silicon carbide (SiC) which is a well-known material in epitaxial graphene synthesis without any harmful chemicals. When SiC substrate is annealed at a very high temperature of around 1500 °C in medium vacuum, its surface is etched and converted into bumpy structure, then GQDs are synthesized on the bumpy structure. The synthesized GQDs are detached from the substrate using a sonication process. As prepared GQD was composed of high quality graphene and had a uniform size and thickness. Size of GQDs grows as the heating temperature decreases, because the higher the annealing temperature promote the sublimation of Si atom and graphene growth rate in vacuum. The photoluminescence signal of pristine GQDs was too weak for using bio-imaging field. However, when additional sonication treatment for 30minutes was performed to as prepared GQDs, the intensity of photoluminescence was dramatically increased. The surface of the GQD was passivated by oxygen functional groups after an additional sonication treatment applied to the GQDs. Furthermore, GQDs after sonication treatment exhibit the size-independent photoluminescence behavior. Thus, it was proved that the surface passivation of GQDs was the dominant photoluminescence mechanism of GQDs. Quantum Yields of photoluminescence is found to be 6.7%. GQDs showed low cytotoxicity and it was observed that cells were maintained in a normal state even after GQDs were injected into the cells.



Poster Presentation : **MAT.P-410**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

A Genetic Protein Design for Self-assembled Adhesive Biomaterials

Pulakesh Aich, An Jaeyeon¹, Joonho Roh^{2,*}, Kyeng Min Park^{3,*}, Kimoon Kim^{4,*}

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Nature exhibits many biomaterials with remarkable chemical and physical properties that often inspire researchers to develop new functional materials. By virtue of remarkable underwater adhesion, mussel foot proteins (Mfps) containing DOPA moieties have been extensively investigated for developing adhesive biomaterials. Although DOPA has been incorporated in numerous biomaterials, the adhesion property of the materials was not as good as that of the natural Mfps in plaques of mussels since the materials were limited to mimic well-defined structure of other Mfps. To overcome this issue, herein, we present a new design of recombinant proteins by genetic insertion of a mussel foot protein (Mfp3) motif into a silk spidroin (MaSp1, showing outstanding mechanical properties attributed by a well-defined beta (β) sheet tertiary structure). The recombinant protein not only self-assembled into a supramolecular fiber, as does the parent MaSp1, but also showed enhanced adhesiveness resulting from the DOPA-containing Mfp3 portion. The successful incorporation of the wet adhesiveness of Mfp3 into the well-structured assembly of MaSp1 provided a new insight for the genetic design of underwater adhesive recombinant proteins by utilizing the structural features of a spidroin protein.

Poster Presentation : **MAT.P-411**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Rapid and Selective Supramolecular Association in Bloodstream

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¹Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Cucurbit[7]uril (CB[7]) is a small-sized synthetic host molecule which has remarkable binding affinity and selectivity towards its specific guest molecules, e.g., adamantanammonium derivatives (AdA) ($K > 10^{14}$ M⁻¹, which is almost comparable to that of streptavidin-biotin). Not only the ultrastable binding affinity between CB[7] and AdA, but also their small-size (~1 kDa), easy-chemical modification, robust chemical structure and scalability were exploited for various bio-applications including biosensors, bioimaging and protein isolations as a replacement of streptavidin-biotin binding pair. To extend its use for biomedical applications such as theragnostic, investigation of their binding ability in a dynamic and complex bloodstream in live animals is highly required. Herein, we demonstrate rapid and selective association of the synthetic binding pair, CB[7]-AdA, in blood flow under an in vivo environment. CB[7]-conjugated tumor targeting antibody and AdA-conjugated fluorescent dye were sequentially injected to tumor bearing mice via an intravenous route. Strong fluorescence signal appeared at a tumor site illustrated that AdA-conjugated fluorescent dye rapidly and selectively bound to CB[7]-antibody accumulated on the tumor. This result successfully indicated that the association of AdA to CB[7] is rapid enough in fast blood flow to detect the target site in mice, which showed great potential of this synthetic binding pair as a new type of chemical tool for biomedical applications.

Poster Presentation : **MAT.P-412**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Surface Modification of Reduced Graphene Oxide and Their Application in Organic Solar Cells as Hole Transport Layer

Jong-jin Park, Dong-Yu Kim^{1,*}

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¹Department of Advanced Materials Engineering, Depa, Gwangju Institute of Science and Technology, Korea

Reduced graphene oxide (rGO) reduced by functionalized hydrazine from GO is promising alternative material to poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) as hole transport layer (HTL) in organic solar cells because it allowed the controllability of electronic properties through versatile functionalization and can improve the long-term stability of solar cells. However, rGO is difficult to apply in inverted organic solar cells because of limited dispersity in alcohol based solvent such as 2-propanol (IPA). Therefore, more research is required about controlling the dispersibility of rGO while maintaining their electrical properties in order that rGO apply to inverted organic solar cells as a HTL via solution process. In this study, we introduced trifluoromethoxy group on the rGO surface (FMrGO) for controlling the dispersibility of rGO while maintaining their electrical properties. FMrGO is well dispersed in IPA and 2-ethoxyethanol due to the flexible methoxy groups. The structural, optical, and thermal properties of FMrGO was characterized by Infrared spectroscopy, EA, XPS, UV-vis spectroscopy and TGA and their work function was estimated by UPS. Finally, we introduced the FMrGO film as a HTL on the active film through solution process and investigated the effect of FMrGO on device performance and long-term stability of inverted organic solar cells.

Poster Presentation : **MAT.P-413**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

RNA producing nanoparticles as platform for a high performance RNA interference system

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Department of Chemistry, Myungji University, Korea

RNA interference (RNAi) is a mechanism mediated by small interfering RNA (siRNA) to a target gene. Here we show a novel nanoparticle capable of producing siRNA and interfering protein expression. The RNAi efficiency of the nanoparticle has been confirmed by GFP activity assay and quantification of RNA production. We have further applied the nanoparticle to GFP expressing live cells and have successfully confirmed the effect of interfering the expression of GFP by measuring the reduced fluorescence intensities. This nanoparticle functioning like a nucleus will provide a novel platform technology for a highly efficient RNAi system. We observed that the siRNA transfection efficiency and the interference effect on mRNA was 7.3 times and 7.9 times higher, respectively when the new system was applied at in vitro transcription and translation experiment.

Poster Presentation : **MAT.P-414**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

TiO₂/graphene Hybrid with Spherical Hollow Structure for Electrochemical Sodium-ion Storage

Won-Jae Lee, Seung-Min Paek*

Department of Chemistry, Kyungpook National University, Korea

In recent, as the demand of lithium-ion batteries have increased due to the development of electronic devices, the demand for anode materials has also increased. Thus, sodium-ion batteries (SIBs) have highly attracted research interests in scientific and industrial field. The titanium oxide (TiO₂) has considered as anodic material in SIBs due to their electrochemical stability. However, TiO₂ is hardly used in SIBs because it has low electrical conductivity to arise from high band gap energy. Thus, in this study, graphene, well-known its high electrical conductivity, was hybridized via layer-by-layer self- restacking with titanate nanosheets to synthesize TiO₂/graphene hybrid with spherical hollow structure. According the electron microscopic studies, the obtained TiO₂/graphene hollow spheres show that the products were formed with spherical hollow structure. And in the energy dispersive spectroscopy results, the titanium and carbon atoms were homogeneously distributed in TiO₂/graphene hollow sphere. And to confirm the enhanced electrical conductivity, electrochemical impedance spectroscopic (EIS) test was conducted. The EIS results show that the TiO₂/graphene hollow spheres have higher electrical conductivity than bulk TiO₂. The sodium-ion half cell tests show that the obtained TiO₂/graphene hollow sphere has higher specific capacity (~200 mAh/g) and cycling performance at various current rates than bulk TiO₂. The TiO₂/graphene hollow sphere could be used as anodic materials for SIBs with enhanced performance.

Poster Presentation : **MAT.P-415**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Paper-based thermochromic displays

Mary Chuong, Oh-Sun Kwon*, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Recently, paper electronics has become a tremendously attractive field since paper is a good substrate for the flexible printing electronics. Cellulose paper as a low-cost, functional organic and environment friendly material possesses verity novel properties, such as flexible, foldable, cuttable, hydrophilic, printable and flammable, which leads adaptably being used for the flexible circuit board for printing functional materials. Here we present the fabrication of a thermoresponsive paper display. A paper-based color display has been fabricated by the ball-pen printing of silver nanoparticle (AgNP) ink and the screen printing of thermochromatic (TC) ink subsequently on the very rough texture surface of paper. Printed AgNP electrode formed the electrical heater to conduct and radiate the heat almost toward the top-coated TC dye. Colorimetric response of TC film was activated by thermal stimulus via an underneath printed silver heater electrode. This thermochromic ink changes its color as the temperature increases. Additionally, thermal electrical and chemical properties of the TC material and the paper heater have been investigated by using various experiment instruments. We observed the structure change of crystal violet lactone (CVL) dye by using many instruments such as FTIR spectroscopy and UV-Vis spectroscopy.

Poster Presentation : **MAT.P-416**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Steady-state Intraband Transition of Ag₂Se Colloidal Nanocrystals

Mihyeon Park, Dongsun Choi, Yunchang Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

The steady-state intraband transition of colloidal quantum dots was reported only in the mercury chalcogenide colloidal quantum dots. Due to the high toxicity of the mercury compounds, it is essential to replace the mercury with a non-toxic material that exhibits steady-state intraband transition. The Ag₂Se nanocrystals show the mid-IR absorption peak similar to that of HgS which is isolated from other transitions. Therefore, the Ag₂Se nanocrystals are synthesized and the mid-IR intraband transition was investigated through spectroelectrochemistry, photoluminescence, and transfer characteristics of the Ag₂Se/ZnO thin film transistor. The spectroelectrochemistry measurement demonstrates that the mid-IR absorption of Ag₂Se nanocrystals is a result of intraband transitions. As the electrochemical reduction proceeds, the mid-IR intraband absorption enhanced at 2201 cm⁻¹, while the NIR band gap transition absorption was bleached at 5485 cm⁻¹. The photoluminescence measurement for the Ag₂Se nanocrystals is the inevitable evidence of the intraband exciton formation. The transfer characteristic of the Ag₂Se/ZnO transistor also shows the proof of the intraband transition of Ag₂Se by generating the photocurrent from IR radiation. The wavelength tunability in the mid-IR region addresses the Ag₂Se nanocrystals are a promising candidate for the wavelength-selective infrared photodetector, infrared filter, and mid-IR laser.

Poster Presentation : **MAT.P-417**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Predicting crystal density of high energy materials using deep neural network method

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Department of Chemistry, Hannam University, Korea

¹Agency for Defense Development, Korea

Explosion is chemically associated with the high rate of reaction in a particular system, and physically, it is the proliferation of energy or matter under certain circumstances, spreading them out of control. The density of high energy material is closely related to Explosion(detonation) velocity and pressure. Synthesis and experiments of high energy material require a lot of attention due to the risk of explosion. In this study, we aimed to predict the density of high energy materials at 25 °C, which is an important factor in explosive performance, through using the structure of the compounds by the Quantitative Structure-Property Relationship (QSPR) method.

In this study, crystal density data were collected from The Cambridge Crystallographic Data Centre (CCDC) and the last 8624 data were obtained from de-duplication, inorganic removal, and abnormal structure removal. The final data is divide into a training set(50%) and a test set(50%), and calculated 604 descriptors through the PreADMET Program. Finally, the model was developed using 172 descriptors through the pre-filter process of Rapid Miner Program. The QSPR model was developed by using multiple linear regression (MLR), support vector machine (SVM), and deep neural network (DNN) methods and we tried to optimized DNN parameters such as rho, epsilon and mini-batch, dropout ratio and activation function. All three models exhibit excellent prediction performance and low error rates, so these models can predict the density of new high energy materials.

Poster Presentation : **MAT.P-418**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation of RuO₂ nanoparticles on CNTs for the degradation of methylene blue

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Department of Chemistry, Chonnam National University, Korea

Homogeneous catalysts are generally very active, but suffer from their high cost and severe activity degradation resulting from poisoning by contaminants. Thus, highly efficient heterogeneous catalysts have emerged as promising alternative strategies due to their easy separation and recycling from the liquid reaction system. Carbon nanotubes (CNTs) have received of attention for supporting material due to their outstanding physical and chemical properties, such as the ultra-high surface area, high mechanical strength, and also high chemical and thermal stability. Ruthenium oxide (RuO₂) has been well known as an effective catalyst for oxygen evolution and transparent electrodes, but the use of RuO₂ nanoparticles in photocatalysis is rarely reported. In this study, we synthesized RuO₂ nanoparticles decorated CNT by introducing thiol groups on CNTs. The prepared catalysts were investigated by means of transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). Also, the photocatalytic activities in the degradation of methylene blue (MB) under UV irradiation were assessed.

Poster Presentation : **MAT.P-419**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Aqueous-phase synthesis of metal hydroxide nanoplates and platinum/nickel hydroxide hybrid nanostructures and their enhanced electrocatalytic properties

Euiyoung Jung, Jinheung Kim^{1,*}

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We successfully synthesized transition metal hydroxide (Ni(OH)₂ and Co(OH)₂) nanoplates in an aqueous solution. These nanoplates have a hexagonal shape with 45nm and 500nm size for Ni(OH)₂ and Co(OH)₂, respectively, from the scanning electron microscopy(SEM) and the transmission electron microscopy(TEM) images. Also, we checked the main growth direction of Ni(OH)₂ and Co(OH)₂ by using the X-Ray diffraction(XRD) results. In addition, we could synthesize platinum/nickel hydroxide hybrid nanostructures (Pt/Ni(OH)₂) in an aqueous solution. The TEM studies of the Pt/ Ni(OH)₂ hybrid nanostructures revealed that a number of 3 nm-sized Pt nanoparticles were well dispersed on the surface of each Ni(OH)₂ nanoplate. The ratio of Pt and Ni(OH)₂ could be readily controlled by using different amount of Pt precursor. We measured the zeta potential values of Ni(OH)₂ to demonstrate the grow mechanism of Pt nanoparticles on the surface of Ni(OH)₂. The Pt/Ni(OH)₂ hybrid nanostructures exhibited enhanced electrocatalytic properties due to synergetic effect of Ni(OH)₂ and Pt. After catalytic reaction, the TEM image and energy dispersive spectroscopy(EDS) of the Pt/Ni(OH)₂ hybrid nanostructures showed unchanged morphology of Ni(OH)₂ nanoplates with Pt nanoparticles, indicating stable materials under electrocatalytic atmosphere.

Poster Presentation : **MAT.P-420**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

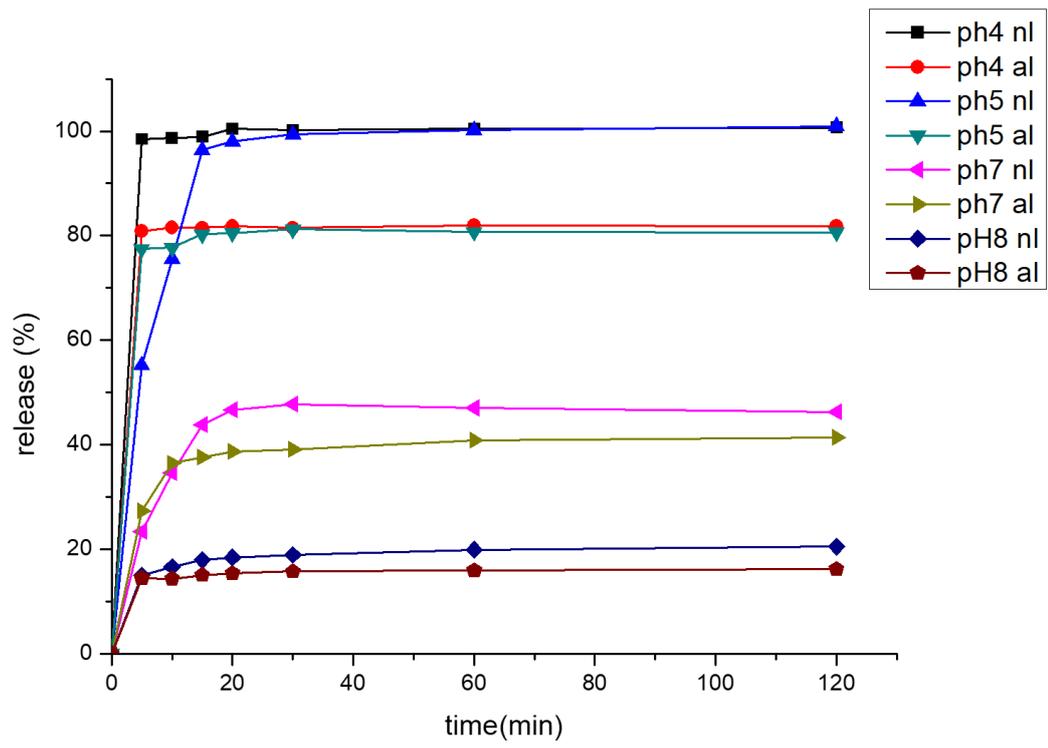
High-Efficiency Mesoporous Hydroxyapatite Nanoparticles For Drug Release using a BSA to a template

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¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Hydroxyapatite[HA,Ca₁₀(PO₄)₆(OH)₂] is an inorganic materials that constitutes the bone supporting the human body. When synthesizing HA, it has various morphologies. Especially, mesoporous HA nanoparticles(MHANS) is suitable for use as an artificial bone. Because HA can load and release a variety of drugs by controlling pore size. In the synthesis of MHANS, the template is mainly Pluronic P123, Pluronic F127, Cetyltrimethylammonium bromide(CTAB) and mono-alkyl phosphate(MAP). In this experiment, bovine serum albumin(BSA) was used as well as CTAB. BSA and CTAB can work together as a template. MHANS using BSA and CTAB as templates together have better properties than MHANS using only CTAB as template. In the wash process, HA that does not use BSA will lose its structure, but HA with BSA will exhibit better characteristics because BSA does not wash out and supports the structure. Levofloxacin(LVF) was loaded on MHANS to measure drug release. Release experiments were performed in pH 4, pH7, and pH 10 buffer solutions to observe the release by pH. Since the HA is degraded at low pH, the drug will be released more effectively and even if the HA is not degraded, the LVF is expected to be differentially released depending on the pH because it is a zwitterion type drug.



Poster Presentation : **MAT.P-421**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Electrocatalytic oxidation of formaldehyde on PtRu-CNTs

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Platinum (Pt) is generally the most active electrocatalyst for oxidation of formaldehyde. However, applications of Pt are hindered because of its high cost and severe activity degradation resulting from poisoning by contaminants. Recently, many attempts have been made to synthesize new types of bimetallic Pt nanostructures (e.g., PtPd, PtCo, and PtRu) for improved catalytic activity and utilization efficiency of the Pt metal. In this study, we report a simple and effective process to prepare PtRu nanoparticles-decorated CNTs (PtRu-CNTs) by using thiolation method on CNTs surfaces. Thiol groups were utilized as linkers to secure the Pt and Ru nanoparticles without agglomeration. The sample was characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The PtRu-CNTs exhibits higher activity in electrochemical reactions of formaldehyde oxidation than that of the reference systems. This synthetic approach should be broadly applicable for preparing CNTs-supported metal catalysts and markedly improves the catalytic activity.

Poster Presentation : **MAT.P-422**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

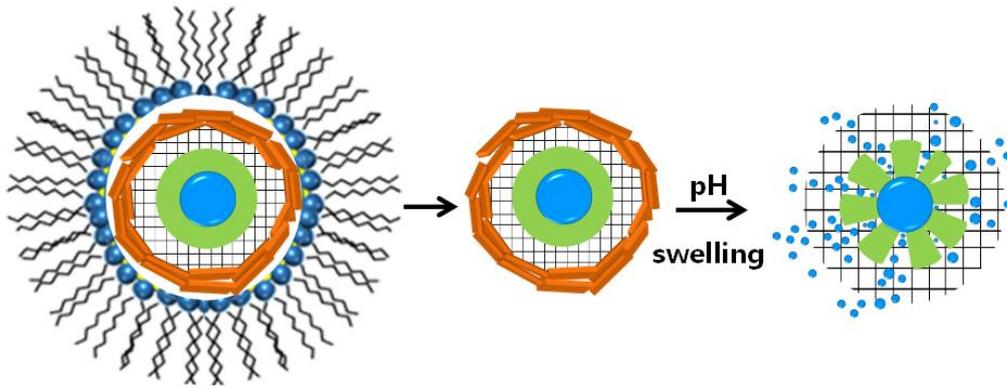
Release of biocompatible inorganic ceramic/pH responsive polymer with crosslinked chitosan in reverse microemulsion

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Inorganic ceramic/pH responsive polymer hybrid nanoparticles synthesized with reverse microemulsion method were prepared to release their contents. Biocompatible and pH-sensitive polymers and layered double hydroxide (LDH) form the hybrid nanoparticles by coating the polymers with LDH. In reverse micelle synthesis, ratio of water to surfactant (W0) is a important factor in controlling morphology and size of nanoparticles. Scanning electron microscopy (SEM) confirmed that the size of hybrids was 50-100 nm and its sphere shape. Chitosan and Eudragit L100 were used for the pH condition of release. Their concentration and crosslinking density of chitosan by glutaraldehyde adjusted the release. Hybrids were the most swelled in acidic conditions. The release of alcian blue through UV/vis spectrophotometer was also higher in acid than in neutral pH 7. The lower the amount of crosslinking, the higher the amount of alcian blue was released under the same pH conditions and the concentration of glutaraldehyde can control burst release of contents.



Reverse emulsion

Poster Presentation : **MAT.P-423**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Application of the deep neural network and machine learning methods for predicting the volume resistivity of polymer composites

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Polymer composite are composite materials made by mixing one polymer material with another polymer material, organic structure, and inorganic materials. Important properties of composites include strength and stiffness, corrosion resistance, fatigue life, abrasion resistance, impact properties, heat resistance, electrical conductivity, insulation, light weight, and appearance. Among them, we tried to develop a model for predicting the volume resistivity, which represents the electrical properties of the material, through the composition ratio between the materials of the polymer composite material. Optimizing the physical properties of composites for various composition ratios is time consuming and costly. Therefore, prediction models of the volume resistivity for the polymer composite material were developed using various machine learning methods that utilize the correlation between composition ratios. The data used in the development of the model were the compound composition and physical property data of polymer composite materials collected from literature and patents, which have been collected by the chemical material solution center in KRICT for several years. The electrical properties data of 352 species obtained from 20 types of materials were divided into 211 species as training set and 141 as external set. The predictive models were developed using multiple linear regression, support vector machine, and deep neural network. The deep neural network method were the most predictive, and the network, hidden layer, dropout ratio, activation function were considered to optimize the results. The developed model developed is expected to be a breakthrough alternative that can save time and cost of developing polymer composites by optimizing material composition with desired electric properties.

Poster Presentation : **MAT.P-424**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

SBA-15 supported Ni(II)-bpy based heterogeneous catalyst for ethylene dimerization

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For several decades, meso-porous silica materials (MPSMs) such as MCM-41 and SBA-15 have attracted much attention for various applications because of their well-ordered pores and large surface area. Although many preparations of silica materials have been reported, controlling their property to fit various applications is important for their use, such as support for heterogeneous catalysts. Therefore, we assume that silica having properly modulated pore size and population of active catalysts may affect the catalytic reaction such as selective generation of alpha-olefin. Particularly, selective creation of 1-butene is biggest task due to their high demand in the industrial applications. Therefore, we prepared SBA-15 containing 4 nm of mean pore diameter and bispyridine grafted, in which we further decorated with various concentration of Ni(II). Interestingly, we have found dramatic changes on reactivities with Ni(II) loading densities. In this presentation, we like to demonstrate their reactivity changes versus Ni(II) loading densities.

Poster Presentation : **MAT.P-425**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

In-situ synthesis of BiOCl_x/BiOBry/BiOI_z decorated on polyacrylonitrile based nanofibers for visible-light photocatalytic investigation

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In this work, BiOCl_x/BiOBry/BiOI_z/PAN (x+y+z=1) composite nanofibers are prepared by electrospinning and sol-gel method. The photocatalytic degradation of trichloroethylene (TCE) over BiOCl_x/BiOBry/BiOI_z/PAN nanofibers were investigated by gas chromatography method. Obtained from results, the optimum photocatalytic activity was achieved with BiOCl_{0.3}/BiOBr_{0.3}/BiOI_{0.4}/PAN fibers under visible light irradiation. From X-ray photoelectron spectroscopy (XPS) result, peaks of C-O, C=O at 286.0 eV, 288.3 eV can disclose that BiOCl_x/BiOBry/BiOI_z has doped on PAN fibers. As for X-ray diffraction (XRD), it can be further confirmed that we had synthesized the as prepared composite nanofibers successfully.

Poster Presentation : **MAT.P-426**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation of graphene quantum dots through hydrothermal method

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Graphene quantum dots (GQDs) has received increasing attention in the past few years owing to its remarkable electronic and physicochemical properties associated with quantum-confinement and edge effects. High conductivity and large specific surface area of GQDs in conjunction with the various active sites on the planar surface render it a desirable and multifarious platform to integrate with diverse nanostructured materials for energy conversion, environmental remediation, and catalysis. In this study, we synthesized GQD from the oxidation of natural graphite powder by a hydrothermal method. By top-down approach because it is much easier to uniformly control the size. The GQDs were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Raman, and ultraviolet-visible (UV-vis) spectroscopy techniques.

Poster Presentation : **MAT.P-427**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation of a New Chromium Thiophosphate Cluster via Solid and Solution State Routes.

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¹Department of Chemistry, Ajou University, Korea

The new chromium thiophosphate cluster, $[\text{PPh}_4^+]_2[\text{Cr}_2\text{P}_2\text{S}_8(\text{H}_2\text{O})_4][\text{Cl}^-]_2[\text{H}_2\text{O}]_{10}$ has been solubilized and stabilize through reactions in water from the chromium thiophosphate precursor, Cs_2CrPS_6 prepared at high temperature via solid state reactions. The crystal structure has been determined by single crystal X-ray diffraction techniques. Cs_2CrPS_6 consists of an alkali metal ion, Cs^+ and a cluster anion, $[\text{CrPS}_6]^{2-}$. The ionic bond in Cs_2CrPS_6 is not stable in polar solvents and they are usually soluble in polar solvents. In this presentation, the alkali metal cations have been replaced by monovalent organic counter cations, $[\text{PPh}_4^+]$. As a result, the title compound crystallizes in the space group $P-1$ and each phosphorus atoms are surrounded by four sulfur atoms in the tetrahedral geometry and chromium atoms are coordinated by four sulfur atoms and two water molecules in the octahedral fashion. These polyhedra are combined to form the dimeric cluster, $[\text{Cr}_2\text{P}_2\text{S}_8(\text{H}_2\text{O})_4]$. Organic cations $[\text{PPh}_4^+]$, halide ions $[\text{Cl}^-]$, and crystal water are included in the crystal via ionic interactions or hydrogen bonds.

Poster Presentation : **MAT.P-428**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

In-situ growth of Graphene Oxide/BiOCl decorated on polyacrylonitrile based nanofibers and their application in photocatalytic degradation of RhB

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¹Department of Chemistry, Inha University, Korea

In this paper, we prepared the graphene oxide/BiOCl/PAN nanofibers by two-step synthesis method and characterized their structures, morphologies, and photocatalytic behaviors by X-ray diffraction, diffuse reflectance spectroscopy, scanning electron microscopy and photocatalytic activity measurements, respectively. From the results, we can obtain that coupling graphene oxide/BiOCl fibers could enable better photocatalytic performances as compared to that pure BiOCl towards the degradation of rhodamine B under visible light irradiation. It could be attributed to the more effective separation of photogeneration electron and holes between BiOCl and graphene oxide, and the better adsorption capacity of rhodamine B.

Poster Presentation : **MAT.P-429**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Influence of Titanium Dioxide on Photocatalytic of Polyvinylpyrrolidone based nanofibers Synthesized via Electrospinning

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In this study, Polyvinylpyrrolidone (PVP) had been chosed as a promising material for electrospun, because it has many desirable properties, such as solubility in various solvents, physiological compatibility, chemical inertness, and excellent film-forming ability. Meanwhile, PVP nanofibers containing titanium dioxide (TiO₂) were synthesized via electrospinning. The photocatalytic activities of the samples were investigated by monitoring the degradation of methylene blue with the samples as photocatalyst under irradiation. The optimum photocatalytic activity was achieved with the webs containing 7 wt% TiO₂. The results showed the proposed method to be effective for improving the photocatalytic properties of TiO₂-doped nanofibers; the doping process also increased the surface area of the nanofibers.

Poster Presentation : **MAT.P-430**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Incorporating Zirconium-Based Metal-Organic Frameworks into Hole Transport Layer for Efficient Organic-Inorganic Solar Cells

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Metal-organic frameworks (MOFs), which are porous coordination polymers exhibiting long-range ordered metal clusters connected with organic linkers, have been studied actively due to their potentials for various applications such as gas separation, drug delivery, catalysis and chemical sensing. There are some of reports expecting that MOFs could be utilized to electronics, but a few reports regarding to MOF-included electronics have also appeared. Among them, organic-inorganic solar cells have risen as promising candidates for photovoltaics (PVs) owing to their superior properties such as effective cost, and use of renewable power source. In order to obtain higher power conversion efficiency of PV devices, the suitable engineering of buffer layer as well as that of active layer is needed. Herein, we reported the application of zirconium-based MOFs to hole transport layer in PV devices. Brushing method from precursor solution under hot-substrate condition was employed to build the thin MOFs films, incorporated into PV devices. By this straightforward strategy, the transparent and thin MOF films converted from precursor solution were deposited, development of films and electronic properties of those were analyzed by photoelectron spectroscopy in air (PESA) and found to be appropriate for charge injection and transfer between active and MOF layer. This result indicates that the brushing method could be a promising candidate for preparing MOF films to be able to fabricate MOF-combined electronics.

Poster Presentation : **MAT.P-431**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

3D ceramic printing of fabricating micro-furnace for lab-on-a-chip

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Department of Chemistry, Sogang University, Korea

Lab-on-a-chip is a more comprehensive concept in microfluidics, which aims to reduce in scale all of the elements of the chemical and processing worlds. This scaling down involves flow and transport necessary for multiple chemical analyses, mixing, detection, separation, and so on. However, it has been challenging to fabricate micro scale high-temperature reactor in microfluidics. Thermally and mechanically strong ceramics have long been used in a variety of machine parts from ancient to now but it was challenging to make micro-scale precision parts with. The fabrication of precise ceramic components offers variable possibilities for experimentation, especially in lab-on-a-chip, where high temperatures are required. The 3D-printed ceramic micro-furnace enables such ultra-high-temperature experiments to be performed at a finer scale, and can also be used in conjunction with other microfluidic devices for a variety of applications.

Poster Presentation : **MAT.P-432**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Catalytic activities of Ni(II)-bpy based porous organic polymers with various Ni(II) loading concentrations

Jongho Yoon, Suk Joong Lee^{1,*}

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¹*Department of Chemistry, Korea University, Korea*

Porous materials are one of the most attractive substances in various areas of industry due to their unique property in porosity and large surface area. Particularly, heterogenization of molecular catalyst by using these porous materials has many advantages in separation, recyclability and stability, although they have relatively lower catalytic activity compared with homogenous counter parts. In previous research, our team report on a new type of Ni(II)-containing porous organic polymer prepared for ethylene dimerization *via* a “click reaction” with tetra(4-azidophenyl)methane and 5,5'-diethynyl-2,2'-bipyridine, followed by metallation with NiCl₂·6H₂O. It showed outstanding catalytic activity toward 1-butene generation with high intrinsic activity as well as high selectivity of 1-butene. However, the generation of long alkyl chain polymer as side products have still remained a challenge. So we tried to make a new concept to overcome this limitation with various Ni(II) loading concentrations in upper mentioned POP. Therefore, we like to present the effect of Ni(II) loading densities in the catalytic activity of Ni(II)-bpy based POP during the ethylene dimerization reaction.

Poster Presentation : **MAT.P-433**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Two-Photon In Vivo Imaging with Porous Silicon Nanoparticles

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College of Medicine, Kyung Hee University, Korea

Fluorescence based bio-imaging technics provide many advantages such as high sensitivity, cost-effective, simple operation, non-invasive, and rapid visualization. The confocal laser scanning fluorescence microscopy (CLSM) is generally used to bio-imaging of biological samples. However, CLSM allowed imaging only a few tens of micrometers for tissues due to the scattering of light and interference of tissue autofluorescence from intrinsic fluorophores. To overcome these issues, two-photon microscopy (TPM) have been developed which show both improved penetration depth and spatial resolution owing to the decreases in tissue autofluorescence and scattering involved with the longer wavelengths (650-1000 nm) of both the exciting and emitting lights. In this study, we presented a porous silicon (pSi) nano-formulation that having high two-photon absorption cross-section value, near-infrared (NIR) photoluminescence emissive, high photo-stability, and high quantum yield. In further study, cancer targeting peptide was functionalized on the surface of pSi, and its TPM bio-imaging was performed in a live xenograft animal model. This study represents the first example of TPM imaging of pSi nano-formulation in live animals and has observed the selective accumulation in disease site.

Poster Presentation : **MAT.P-434**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

***Ab-initio* calculations on Al-doped SrTiO₃**

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SrTiO₃ (STO) is regarded as a representative high-k material in oxide electronics, owing to its high mobility and dielectric constant (~300). However, because of its n-type nature and relatively small band gap (3.3 eV), Schottky barrier between the metal-STO interface is under 1 eV, which leads to large leakage current. It has been repeatedly reported that the intrinsic n-type nature of STO originates from thermodynamically stable oxygen vacancy. The most straight forward approach to control the Fermi level of STO is the acceptor doping, which reduces the n-type carrier concentration and hence increases the Schottky barrier. There have been many studies about the effect of extrinsic dopant on STO, and it was found that the doping of Fe or Cr ions at Ti sites reduces the leakage current significantly. Even though it is expected that Al doping on STO should give similar behavior, the detailed analysis with regard to the doping effect has been hardly carried out. In this study, first-principles calculation on Al dopant in STO is carried out. The defect formation energies including intrinsic defects are calculated with hybrid density functional method. The concentration of each defect configuration and the position of the Fermi level is found. This study will give a meaningful insight into the designing of oxide electronic devices.

Poster Presentation : **MAT.P-435**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Hollow Structured Graphene with Impregnated Mn₃O₄ for Lithium-ion Battery Application

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In the field of batteries, graphene has received enormous interests owing to its large specific surface area and excellent electrical conductivities. And the manganese oxide has low electrochemical conversion potential, small bending stresses, and large theoretical capacity. So, we attempted to hybridize graphene with manganese oxide to obtain high synergetic effects such as higher capacity by adding manganese oxide. According to the electron microscopic study, the synthesized graphene/manganese oxide nanohybrids had spherical hollow structure, and their energy dispersive spectroscopic mapping images showed that the manganese oxide nanoparticles were homogeneously distributed in graphene hollow sphere. In the electrochemical impedance spectroscopy, the graphene/manganese oxide nanohybrid had high electronic conductivity and ion-diffusion property. Electrochemical lithium-ion storage tests showed that the obtained nanohybrids had larger specific capacity than the bare graphene. The graphene/manganese oxide nanohybrids could be used as anodic materials in lithium-ion batteries.

Poster Presentation : **MAT.P-436**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Co-assembly and Charge-transfer Characteristics of Porphyrin Box (PB)@Fullerene Supramolecular architectures

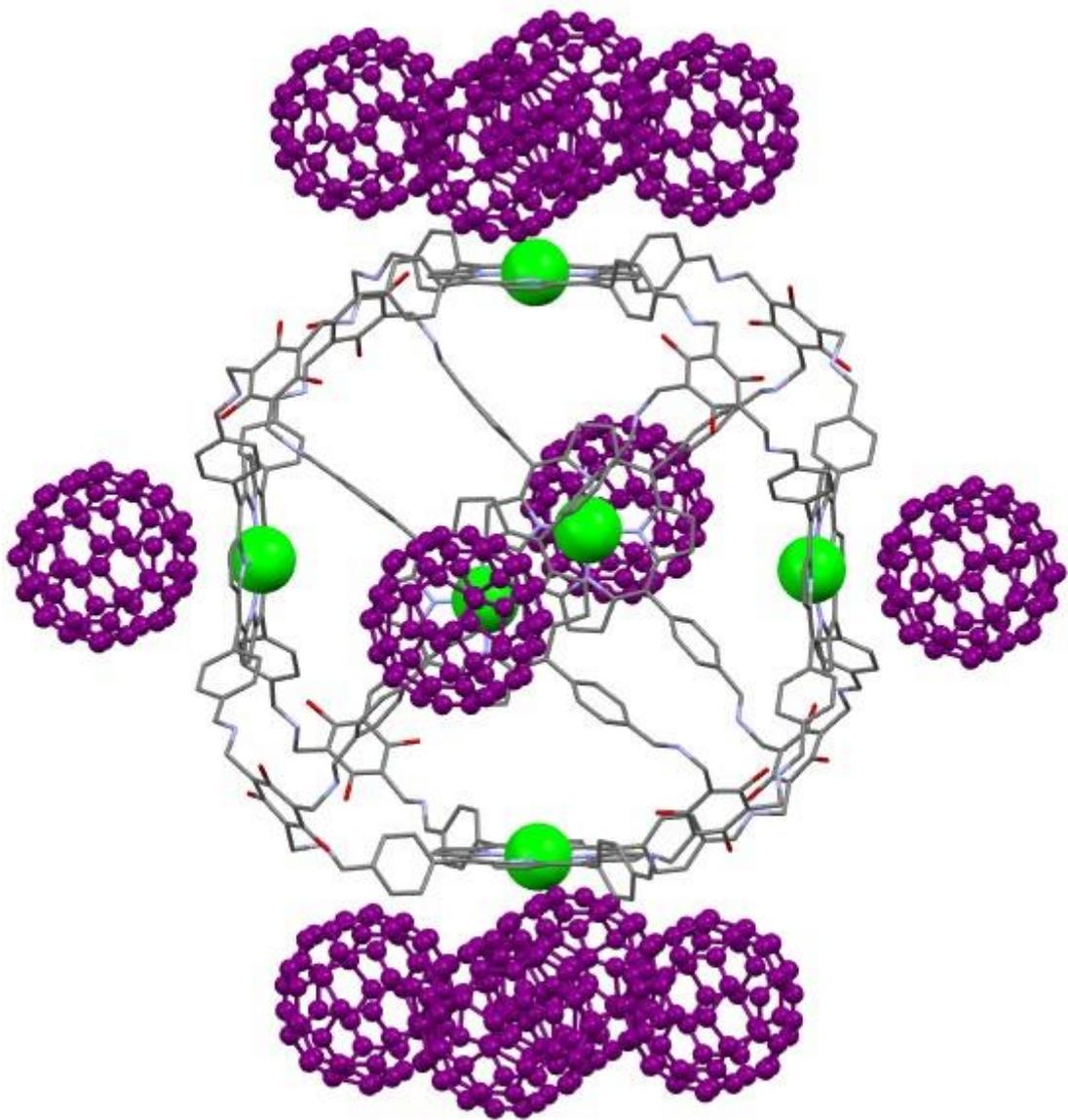
Xiujun Yu, Younghoon Kim¹, Jaehyoung Koo¹, Ikjin Kim², In-Chul Hwang^{1,*}, Kimoon Kim^{1,*}

Center for Self-assembly and Complexity, Institute for Basic Science, China

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Due to outstanding electron donating features of porphyrins and unique electron accepting properties of fullerenes, various supramolecular porphyrin-fullerene architectures have been reported for the applications in the emerging fields of optoelectronics, molecular wires, bioenergetics and solar cell transducers.[1-4] Herein, we developed a series of novel porphyrin@fullerene donor-acceptor supramolecular architectures (Fig. 1) by using a porous porphyrin cage and fullerenes. The porphyrin cage, known as porphyrin box (PB), which has a cavity of 1.95 nm in diameter[5] contains six porphyrin moieties. The optoelectronic properties of the supramolecular assemblies are tunable by functionalizing the pores of porphyrin boxes and the number of fullerenes can be controlled by regulating the co-crystallization conditions.



Poster Presentation : **MAT.P-437**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Effect of Graphene Nanoparticles on High performance Dental Resin Cement Material

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Department of Optometry, Daegu Catholic University, Korea

The purpose of this study was to investigate the effects of BIS GMA (Bisphenol A glycerolate dimethacrylate), HPMA (Hydroxypropyl methacrylate), diluent TEGDMA (Triethylene glycol dimethacrylate) and Camphorquinone as photoinitiator, and Graphene oxide nanocolloids as additive. And also, the polymerization time and the viscosity of the sample were compared with the basic dental resin cement. HPMA was added at 80%, 100% and 120%, respectively, based on BIS GMA. Graphene oxide nanocolloids were extracted from each group with 0.05% and 0.1%, respectively. The viscosity of the sample was measured, and the polymerization of the sample proceeded to visible light of about 460 nm. The polymerization time was selected based on optimal curing conditions. First, 80% REF samples with the least amount of HPMA were the shortest in 20 seconds and increased to 30-40 seconds as the proportion of HPMA increased. With the addition of graphene particles, samples with 80% HPMA increased from 50 to 60 seconds, samples with 100% increased to 60 to 70 seconds, and samples with 120% increased to 70 to 80 seconds. The viscosity of the sample was increased from 790 to 800 cp as compared with 150 to 170 cp of Ref sample. Considering the viscosity of the sample and the polymerization time, the group with 80% of HPMA and 0.1% of Graphene particles were most suitable for use as the most dental resin cement.

Poster Presentation : **MAT.P-438**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthetic routed to superparamagnetic Fe₃O₄@SiO₂@TiO₂ spheres through one-step solvothermal method

Eunmi Im, Hojun Seo, Geonda Moon*

Korea Institute of Industrial Technology, Korea

Manipulation of the initial structures of nanocrystals is desired to integrate the ability to harness the size-dependent properties of individual nanocrystals with the possibility to control collective properties due to interactions between the subunits. Herein, we report the synthetic method for controlling the superparamagnetic Fe₃O₄@SiO₂@TiO₂ colloid size based on solvothermal process. The water-soluble superparamagnetic Fe₃O₄ colloidal nanocrystal clusters(CNC) with uniform size range from about 30 to 200 nm. Metal oxides can be coated on magnetite colloidal nanocrystal clusters to protect the superparamagnetic nature of magnetite nanocrystals from phase change.

Poster Presentation : **MAT.P-439**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Synthesis and Structure of the New Mixed-metallic Sulfide, $\text{Rb}_y(\text{Fe}_x\text{Ge}_{2-x})\text{Ge}_8\text{S}_{20}$.

SangHyun Bae, Woojin Yoon, Hoseop Yun^{1,*}

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¹*Department of Chemistry, Ajou University, Korea*

The new mixed-metallic sulfide, $\text{Rb}_y(\text{Fe}_x\text{Ge}_{2-x})\text{Ge}_8\text{S}_{20}$ has been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. The title compound crystallizes in the space group $P2_1/a$. The title compound is isostructural with the previously reported compounds, $\text{Rb}_3\text{Al}_3\text{Ge}_7\text{S}_{20}$ and $\text{K}_3\text{Ga}_3\text{Ge}_7\text{S}_{20}$. There are five crystallographically independent Ge sites surrounded by four sulfur atoms in the tetrahedral fashions. One of the Ge sites is partially occupied by statistically disordered Ge and Fe atoms.

Poster Presentation : **MAT.P-440**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Characterization of hydrogel lens materials containing cerium oxide nanoparticles

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The purpose of this study was to analyze the physical characteristics of ophthalmic lenses that were manufactured using cerium oxide nanoparticles as additives to increase UV blocking effect of ophthalmic lenses. In this study, cerium oxide was used to copolymerize with the basic monomer HEMA (2-hydroxyethyl methacrylate), the cross-linker agent (ethylene glycol dimethacrylate) and initiator (azobisisobutyronitrile). Also, the optical and physical properties such as spectral transmittance, water content, contact angle and breaking strength of the prepared lens were measured. The physical and optical properties of the manufactured hydrogel lens were compared with the Ref without additive. The results showed that the water content was maintained and the contact angle and tensile strength increased with the additive ratio, the contact angle increased by 4.32 ~ 15.19% and the strength increased by 41.58 ~ 55.55%. Also, ultraviolet transmittance was greatly decreased with increasing additive ratio. Cerium oxide is expected to be useful as a material for manufacturing hydrogel lenses that increase contact angles and strength without changing the properties of the water content, and have excellent UV protection.

Poster Presentation : **MAT.P-441**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Cycling Performance of Lithium Ion Batteries Using Morphology- Controlled WO₃ and WS₂ Nanocrystals

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As a promising candidate for anode materials in lithium ion battery (LIB), tungsten trioxide (WO₃) and tungsten disulfide (WS₂) nanocrystals were synthesized, and their electrochemical properties were comprehensively studied. WO₃ nanowires by hydrothermal methods, and WS₂ nanosheets by unique gas phase sulfurization of WO₃ using H₂S. WS₂ nanosheets exhibits uniformly 10 nm thickness. The WO₃ nanowires and WS₂ nanosheets showed a maximum capacity of 552 and 633 mA h g⁻¹ after 100 cycles after 100 cycles. Especially, the capacity of WS₂ is significantly larger than 433 mA h g⁻¹. We also examined the cycling performance using a larger size WO₃ and WS₂ nanocrystals, showing that the morphology and size of nanocrystals plays an important role in determining the capacity of LIBs. The size effect is ascribed to the lower charge-transfer resistance between the nanosize surface and electrolyte.

Poster Presentation : **MAT.P-442**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Mineralization of Indigo Carmine using $\text{ZnBi}_2\text{O}_4\text{-Bi}_2\text{S}_3$ composites under visible light radiation

Huy B.t., Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

Indigo carmine (3,3'-dioxo-2,2'-bis-indolyden-5,5'-disulfonic acid disodium salt) or acid blue 74 is one of the widely dyes used in the textile industry. The high toxicity of Indigo carmine may lead to potentially dangerous increase in blood pressure, disturbances in the reproductive, and neuronal systems. Indigo Carmine was mineralized under visible light irradiation using novel $\text{ZnBi}_2\text{O}_4\text{-xBi}_2\text{S}_3$ photocatalysts, which was prepared by a hydrothermal method. The results showed that photocatalytic activity of the $\text{ZnBi}_2\text{O}_4\text{-Bi}_2\text{S}_3$ composites was greatly enhanced (~ 20 times) in compared to that of pristine ZnBi_2O_4 . The synergetic effects, charge transfer between ZnBi_2O_4 and Bi_2S_3 , as well as the separation efficiency of the photogenerated electrons and holes may be reasonable of photocatalytic activity enhancement. The superoxide anion radical was the major active species responsible for the photodegradation process. These results demonstrate the feasibility of utilizing $\text{ZnBi}_2\text{O}_4\text{-Bi}_2\text{S}_3$ as potential photocatalyst.

Poster Presentation : **MAT.P-443**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Eu-doped Bi₂WO₆ for the photodegradation of 2,4,5-Trichlorophenoxyacetic acid.

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Photocatalyst is considered to be a qualified candidate and has been attracting much attention for the degradation of toxic organic pollutants environment-friendly under light expose. The tungstate based materials such as Y₂WO₆, CaWO₄ ZnWO₄ and Bi₂WO₆, have been investigated widely for their electric, optical and environmental applications. 2,4,5-Trichlorophenoxy acetic acid (2,4,5-T) is one of the most widely used herbicides which cause irretrievable damage to the environment. We prepared Eu-doped Bi₂WO₆ by one-step hydrothermal method. The morphologies were characterized by using XRD, XPS, and SEM. Results show that Eu-doped Bi₂WO₆/H₂O₂ system exhibits high photodegradation performance for 2,4,5-T. The effects of dopands, H₂O₂, and pH on photodegradation were investigated and the stability and available reusability were also evaluated. Keywords: Photocatalyst, 2,4,5-Trichlorophenoxy acetic acid, degradation

Poster Presentation : **MAT.P-444**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Novel molecularly imprinted polymer for the detection of cancer biomarker

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Herein, we integrated the high selectivity from boronate affinity binding with the extraordinary signals, stability, and biocompatibility from conjugated polymer for the development of novel label-free alpha-fetoprotein (AFP) sensor. The proposed molecular imprinted polythiophene sensor displayed a high sensitivity, low detection limit, wide detection range, good selectivity, acceptable reproducibility and satisfying stability. In addition, this sensor was successfully applied for the determination of AFP in human saliva samples. Besides, our method avoids the use of antibodies, enzymes, nanomaterials for signal amplification or complicated multiple label procedures. With these advantages, this method would provide a wide potential application for other cancer biomarkers detection in clinical diagnosis.

Poster Presentation : **MAT.P-445**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Paper-based analytical devices for sensing folic acid-using Rhodamine B derivatives

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Folic acid (FA), known as Vitamin B9, pteroylglutamic acid (PGA) or folate, is a water-soluble vitamin and has been confirmed as a significant nutrient in humans and animals. A paper-based analytical device (PADs) for the determination of folic acid (FA) was designed using rhodamine B derivative-Cu²⁺ complex as a color indicator. The structural change of rhodamine B derivatives to be the ring-open form (pink color) was enhanced by folic acid. The mechanism is based on the improvement of electron transfer from rhodamine B derivatives to Cu²⁺ in the presence of folic acid. The variation in color intensity can be either tracked by a UV-vis spectrophotometer or PADs. The variation of color intensity in PADs was quantified by using Red, Green, and Blue components (RGB) analysis. The analytical performance of the developed system including linearity, detection limit and reproducibility has been evaluated. The method showed a great potential for determination of folic acid in real samples.

Poster Presentation : **MAT.P-446**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Chemiluminescent probes –based on paper strips for detection of influenza

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According to the World Health organization (WHO), millions of people are infected by influenza virus every year. Traditional diagnosis methods for influenza virus require high cost equipment and technician with time consuming process. During the last decade, the development of alternative diagnosis techniques for influenza has received a tremendous attention of scientists. The emerging paper-based analytical devices (μ PAD) has shown their potential with low cost and easy to use for the detection of several toxic molecules. Moreover, the availability as renewable natural resources of natural cellulose fibers, low cost, recyclability, and the possibility to modify the surface of the paper with sensing molecules such as chemiluminescent/fluorescent probe is promising in the development of novel sensing devices. Unlike fluorescent probes, the emerging chemiluminescent probe do not require light excitation, resulting in higher sensitivities and signal-to-noise ratios. In this work, we aim to develop the paper strips based on Schaap's dioxetane derivative that is responsive to influenza virus.

Poster Presentation : **MAT.P-447**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Highly selective and sensitive detection of TNP in environmental water using based amphiphilic polymer-coated quantum dots

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Novel optical sensor was constructed via a facile in-situ polymerization strategy for highly selective and sensitive detection of trinitrophenol (TNP) in environmental water. We synthesized a series of amphiphilic thiophene monomers with side chains bearing different groups which were used for preparing amphiphilic polythiophene coated CdTe QDs (P1QDs). P1QDs sensor was synthesized by in situ polymerization of amphiphilic thiophene monomer on the surface of CdTe QDs to yield highly fluorescent P1QDs sensor. The emission of the P1QDs is found to be quenched in the presence of TNP by electron transfer mechanism through electrostatic and hydrogen bonding interactions and showed excellent selectivity for TNP over its analogues. P1QDs sensor displayed excellent limits of detection for TNP of 0.56 nmol L^{-1} ($R^2= 0.9946$) with linear ranges of $0.05\text{-}14 \mu\text{mol H}^{-1}$. Furthermore, the sensor was successfully applied to determine TNP in tap and river water samples, presenting high recoveries in the range of 95.5–106.3% and 96.9–110.88% at three spiking levels with the relative standard deviation within 1.54–3–2.32% and 1.44–2.81%, respectively. The simple, rapid, non-toxic P1QDs based method proved potentially applicable for the highly selective and sensitive fluorescent determination of trace TNP in complicated environmental water samples. Keywords: Polythiophene, QDs, trinitrophenol (TNP), river water, electron transfer mechanism

Poster Presentation : **MAT.P-448**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

New fluorescent material from Ginkgo biloba leaves

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Green chemistry field has attracted because of its clean and sustainable feature. The preparation of new fluorescent materials using nontoxic solvents and economical materials gave several advantages for a green synthetic strategy. New fluorescent material was synthesized using a simple hydrothermal method with ginkgo biloba materials (GBM) extracted from ginkgo biloba dried leaves. The separation and quantification of GBM were accomplished using a reversed-phase C18 column with the mobile phase of ethanol and using UV detector operated at 254 nm. We found that rutin, quercitrin, bilobalide, and quercetin dehydrate were dominant in GBM composition. Under an excitation at 350nm, GBM produced high luminescence in the range of 440-450 nm. Our preliminary study would give a potential leading to new natural product synthesis for biological application in the near future.

Poster Presentation : **MAT.P-449**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Cook for future; ultrafast and low-cost synthesis via kitchen microwave oven for multivalent battery materials

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Batteries have become very important in these days for our new future, smartphone, electric vehicle, smart grid and so on. In order to utilize these things, high volumetric capacity and power density are essential. One strategy to prepare future demands is that utilize multivalent ion with earth-abundant materials (Zn^{2+} , Mg^{2+} , Al^{3+} and Ca^{2+}). Multivalent-ion batteries can offer double or triple-times as electrons per metal ion involved in the redox reaction with electrode materials. Therefore, those can offer higher volumetric capacity and energy density than Li-ion batteries. Despite these strengths, not of many active materials have been discovered yet. At this point, there is no choice but to trial and error method for finding materials. Normally, active materials are synthesized by the solid-state, sol-gel and hydrothermal methods. These methods have good yield, but, synthesis takes a quite long time (more than several hours). Time is a very important variable in the trial and error process. To reduce the time for synthesis, we used a commercialized microwave oven for synthesizing battery materials. Microwave heating has these advantages, ultrafast, clean, low cost, energy-effective and also high-yielding. In this study, we synthesized MMo_6S_8 ($M=Cu, Zn, Mg$ and Ca) and various oxide materials for multivalent-ion batteries within several minutes (~ 3mins). We hope this synthesis method will aid not only to discover multivalent-ion battery materials but also to discover various materials.

Poster Presentation : **MAT.P-450**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Thermally treated Ti₃CN MXene with excellent EMI shielding Properties

Aamir Iqbal

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Thermally treated Ti₃CN MXene with excellent EMI shielding Properties Aamir Iqbal^{1,2}, Mohamed Alhabeb³, Yury Gogotsi^{3*}, and Chong Min Koo^{1,4*1} Materials Architecturing Research Center, Korea Institute of Science and Technology (KIST), 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea. 2 Nanomaterials Science and Engineering, University of Science and Technology, 217, Gajung-ro, Yuseong-gu, Daejeon 34113, Republic of Korea. 3 Department of Materials Science and Engineering, and A. J. Drexel Nanomaterials Institute, Drexel University, 3141 Chestnut Street, Philadelphia, PA 19104, USA. 4 KU-KIST Graduate School of Science and Technology, Korea University. Recent advances in electronics and telecommunication have revolutionized the modern era by facilitating the human beings. Meanwhile, this dramatic rise in the number of electronic devices has introduced electromagnetic interference (EMI); a kind of disturbance causing the malfunctioning of the device itself as well as the surroundings. Hence, the materials with outstanding EMI shielding capability with ease of processing are strongly needed. Two dimensional transition metal carbides and/or nitrides have great potential towards EMI shielding application. Here, nitride based Ti₃CN MXene was synthesized and thermally treated at different temperatures followed by vacuum assisted filtration. Electrical conductivity was significantly increased after thermal treatment. Samples were characterized by XRD, SEM, and TEM and finally EMI was measured in the frequency range of 8.2-12.4 GHz (X-band). An excellent EMI shielding efficiency (SE) of over 100 dB at a thickness of 30 micron with absorption dominant characteristics was obtained.

Poster Presentation : **MAT.P-451**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Li-Al-Ge-S systems : synthesis and structure determination for new solid electrolytes of all-solid-state Li batteries.

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All-solid-state Li batteries are next generation battery systems since the higher safety on replacing organic liquid electrolytes. Herein we report novel Li-Al-Ge-S systems for solid electrolytes of all-solid-state Li batteries for the first time. The materials are prepared by mechanical milling of Li_2S , Al_2S_3 and GeS_2 . The powder mixtures were pressed into a pellet, sealed in carbon-coated quartz tubes under vacuum and heated to 750 °C for 10 h. The synthesized materials were confirmed by powder X-ray Rietveld refinement and the Li ion conductivities were measured with the impedance spectroscopy at room temperature. In this work, we will present material synthesis, crystal structure, and the lithium ion conductivity behavior of crystalline materials in Li_2S - Al_2S_3 - GeS_2 systems, demonstrating the materials can be potential solid electrolytes for all-solid-state Li batteries.

Poster Presentation : **MAT.P-452**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Investigation of electrochemical magnesium-ion intercalation mechanism in Ammonium Vanadium Bronze

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Magnesium battery (MBs) has received attention as one of post lithium-ion battery systems because of potential advantages in cost and capacity. However, only a few materials show a capability of magnesium intercalation in a conventional organic electrolyte. Herein, intercalation/de-intercalation capability of magnesium ion into/from $\text{NH}_4\text{V}_4\text{O}_{10}$ is demonstrated for the first time as a cathode material for MBs in a conventional organic electrolyte. The material is synthesized from ammonium hydroxide, vanadium pentoxide, oxalic acid, and hydrochloric acid, using a hydrothermal reaction method at 180 °C for 5 hours, which serves as the working electrode in an electrochemical cell with activated carbon as the counter and reference electrode, and 0.5 M $\text{Mg}(\text{ClO}_4)_2$ in acetonitrile as the electrolyte. The cell shows a reversible magnesium intercalation reaction with the initial discharge and charge capacity of 175 mAh g⁻¹ and 205 mAh g⁻¹, respectively. The capacities are higher than those previously reported for vanadium oxides. The capacity retention at 1 C-rate is 36.8 mAh g⁻¹ at the 100th cycle. The magnesian/demagnesian process is confirmed using elemental analysis, X-ray diffraction and X-ray photoelectric spectroscopy (XPS). These results demonstrate the material as a potential high capacity cathode material for MBs in a non-aqueous electrolyte.

Poster Presentation : **MAT.P-453**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Thermally treated Ti₃CN MXene with excellent EMI shielding Properties

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Thermally treated Ti₃CN MXene with excellent EMI shielding Properties Aamir Iqbal^{1,2}, Mohamed Alhabe³, Yury Gogotsi^{3*}, and Chong Min Koo^{1,4*1} Materials Architecturing Research Center, Korea Institute of Science and Technology (KIST), 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea. ²Nanomaterials Science and Engineering, University of Science and Technology, 217, Gajung-ro, Yuseong-gu, Daejeon 34113, Republic of Korea. ³Department of Materials Science and Engineering, and A. J. Drexel Nanomaterials Institute, Drexel University, 3141 Chestnut Street, Philadelphia, PA 19104, USA. ⁴KU-KIST Graduate School of Science and Technology, Korea University. Recent advances in electronics and telecommunication have revolutionized the modern era by facilitating the human beings. Meanwhile, this dramatic rise in the number of electronic devices has introduced electromagnetic interference (EMI); a kind of disturbance causing the malfunctioning of the device itself as well as the surroundings. Hence, the materials with outstanding EMI shielding capability with ease of processing are strongly needed. Two dimensional transition metal carbides and/or nitrides have great potential towards EMI shielding application. Here, nitride based Ti₃CN MXene was synthesized and thermally treated at different temperatures followed by vacuum assisted filtration. Electrical conductivity was significantly increased after thermal treatment. Samples were characterized by XRD, SEM, and TEM and finally EMI was measured in the frequency range of 8.2-12.4 GHz (X-band). An excellent EMI shielding efficiency (SE) of over 100 dB at a thickness of 30 micron with absorption dominant characteristics was obtained.

Poster Presentation : **MAT.P-454**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

EMI shielding Properties of Conducting Polymer/ 2-D material composite Film

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EMI shielding Properties of Conducting Polymer/ 2-D material composite Film Pradeep Sambyal¹, Jun Pyo Hong¹, Aamir Iqbal¹ and Chong Min Koo^{1,2,*} ¹Center for Materials Architecturing, Korea Institute of Science & Technology, Hwarangno 14-gil 5, Seong-Buk Gu, Seoul, Republic of Korea. ² KU-KIST Graduate School of Science and Technology, Korea University. Advancement of electronics systems has made human life more easy and comfortable, but it has introduced new type of pollution. Electromagnetic pollution exhibits depraved effect on the working of electronic machines and also have adverse effect on human health. So necessity to suppress the impact of EM radiations to complex machineries, living bodies and environment has become essential requirement. Herein we synthesized conducting polymer/2D material composite films through vacuum filtration assisted technique. The obtained composite film were thoroughly characterized using SEM, FTIR, XRD, TGA, and EMI shielding analysis. The synergistic combination of these two material lead to the absorption dominated shielding effectiveness value of 50dB in the frequency range of 8.2-12.4 GHz (X-band).

Poster Presentation : **MAT.P-455**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Li-Zn-P-S System : Sulfide Solid Electrolyte for All-Solid-State Battery

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As many problems have arisen in battery systems recently, safety issues also have received attention. In current systems, liquid organic electrolyte can't solve the dendrite problem of lithium metals. So new system is needed to solve that problem. All-solid-state batteries is one of the candidates for future electrochemical energy storage system. They are expected to be safer than current battery systems due to the reduce of dendrite problems. Moreover, sulfide systems have higher ionic conductivity than oxide materials. Thus, they can obtain similar or higher ionic conductivity of liquid electrolyte. Following such advantages, all-solid-state battery system has received attention in future battery research field. Herein, we introduce Li-Zn-P-S systems as electrolyte candidates for an all-solid-state battery system. In this work, we will present synthesis method and characterization of its crystal structure and electrochemical properties as a solid electrolyte material for all-solid-state battery.

Poster Presentation : **MAT.P-456**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Three-Dimensional Modeling of Quasicrystal Structures by Automatic Approach: An Icosahedral Zn-Mg-Y Alloy

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Quasicrystals (QCs) are long-range ordered but aperiodic crystal, having rotational symmetry of 5-fold. There are some approaches to solve the structure of QCs, such as Penrose tiling or High-dimensional (HD) crystallography, but they are challenging because of its complexity. Here, we report a simple approach to three-dimensional (3D) atomic modeling from X-ray diffraction and solve the structure of icosahedral QC $Zn_{0.50}Mg_{0.42}Y_{0.08}$. The key idea of approach to 3D atomic modeling is to use the observed value (in \AA^{-1}) of the reciprocal vectors in the 3D Cartesian coordinate system without assuming any unit cell. To simplify for larger scale, it is modified to revise the method to be automatic. As a result, there are 25429 atoms within a sphere of $\sim 48\text{\AA}$ radius. Structure motifs with hierarchical natures can be found. Isolated icosahedral clusters with filled center sites are surrounded by concentric dodecahedron. Remarkably, Bergman type clusters which exclude origin are found in this structure. It means the model can be chosen in other region regardless of the inclusion of the origin, or in any size in space without limit, which is one of the properties of quasicrystal. Also, characteristics that clearly distinguish each atom are found, which are well-matched with previous research. The structural model of Zn-Mg-Y alloy is strikingly similar to those obtained via former approaches such as HD crystallography, but show very clear real-space relationships between the clusters.

Poster Presentation : **MAT.P-457**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Crystal Structures of $Zn_xH_2V_3O_8$, Prepared by Electrochemical Intercalation of Zn Ions in Organic Electrolytes

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The crystal structures of $Zn_xH_2V_3O_8$, prepared by electrochemical Zn^{2+} ion intercalation into $H_2V_3O_8$ in organic electrolyte, have been characterized. The electrochemical properties were investigated in homemade cell using 0.5M $Zn(ClO_4)_2$ in AN as electrolyte and Zn metal as counter electrode in 60°C. The structure of $Zn_xH_2V_3O_8$ has been determined and refined for the first time by this work using the technique of structure determination from powder x-ray diffraction data. The space group is P 21/m and a, b, c and β parameters are 16.532 Å, 3.709 Å, 9.368 Å and 90.375°. With the zinc ions insertion from $H_2V_3O_8$ to $Zn_xH_2V_3O_8$, the cell volume and b parameter are increased by 0.3% and 2%, respectively, but a parameter is decreased by 2%. The results would also provide an important basis for understanding other electrochemical intercalation reaction of divalent ions into various host materials.

Poster Presentation : **MAT.P-458**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

New Na superionic conductors $\text{Na}_{4-x}\text{Sn}_{1-x}\text{Sb}_x\text{S}_4$ ($0.02 \leq x \leq 0.33$) for all-solid-state Na-ion batteries: *ab initio* structure determination from powder X-ray diffraction data

Jongwook Heo, Seung-Tae Hong*

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A new structural class of Na superionic conductors $\text{Na}_{4-x}\text{Sn}_{1-x}\text{Sb}_x\text{S}_4$ ($0.02 \leq x \leq 0.33$) with a space group $I4_1/acd$ was discovered in the course of systematic investigation of materials with a range of nominal compositions of $0.0 \leq x \leq 0.5$. The new structure was determined from powder X-ray data, consisting of distinct two types of non-sodium metal sites, Sn-only and Sb/Sn mixed sites in a tetrahedral coordination. The evolution of a new phase, distinctly different from Na_4SnS_4 or Na_3SbS_4 , allows fast ionic conduction in three-dimensional (3D) pathways ($0.2\text{-}0.5 \text{ mS cm}^{-1}$ at $30 \text{ }^\circ\text{C}$). The new $\text{Na}_{4-x}\text{Sn}_{1-x}\text{Sb}_x\text{S}_4$ showed excellent dry-air stability, no H_2S evolution in contact with water, and reversible precipitation from the homogeneously dissolved aqueous solution, highlighting the potential in their practical use. The high capacity and the stable cycling performance of $\text{TiS}_2/\text{Na-Sn}$ all-solid-state Na-ion batteries using $\text{Na}_{3.75}\text{Sn}_{0.75}\text{Sb}_{0.25}\text{S}_4$ were successfully demonstrated.

Poster Presentation : **MAT.P-459**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Vanadium oxide as a new lithium-free cathode material representing remarkable energy density

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Among metallic elements, lithium has low atomic mass (6.94 g mol^{-1}), high specific capacity (3860 mAh g^{-1}), and the most electropositivity (-3.04 V vs. SHE), which facilitate designing of batteries with high energy density. Thus, lithium-ion batteries (LIBs) have been the leading energy storage technology. The initial study of electrochemical Li intercalation into V_4O_9 was reported by A. Hammouche in 1987, and was considered as a cathode material for LIBs by F. Mattelaer et al. in 2016. The charge-discharge properties were evaluated with thin film electrodes comprised of various vanadium oxides, and V_4O_9 has the highest volumetric energy density among the Wadsley series ($\text{V}_n\text{O}_{2n+1}$ — VO_2 , V_2O_5 , V_6O_{13} , V_3O_7 , V_4O_9). Herein, we present V_4O_9 as high performance cathode material for LIBs, and reveal the mechanism of lithiation/delithiation behavior. In order to improve diffusivity and rate capability, the particle size of V_4O_9 was controlled. In addition, the electrochemical stability that adversely affects by the vanadium dissolution problem was improved by adopting an appropriate electrolyte which was compared with the 1M LiPF_6 in EC/DMC, a conventional electrolyte. Based on this approach, we have found that V_4O_9 demonstrated high energy density (270 mAh g^{-1} , 2.6 V) comparable to conventional LiCoO_2 .

Poster Presentation : **MAT.P-460**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Sodium vanadium phosphate as an intercalation based cathode material for calcium-ion batteries

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Calcium-ion batteries (CIBs) is one of the candidate for the next generation battery systems due to their many benefits in terms of energy density and low cost—calcium has a similar redox potential with lithium (Li = -3.04 V, Ca = -2.87 V vs SHE), and the capacity can be doubled by the divalency of the ion compared with monovalent lithium ion. However, there are only a few materials known as a reversible intercalation host of calcium ions. So far, some of known examples are Prussian blue analogues and CaCo_2O_4 . Herein, we report a remarkable new host material as a cathode material for CIBs. It has the NASICON-type structure with an open three-dimensional framework enabling a facile diffusion of calcium ions. Prior to attempting electrochemical calcium intercalation, we have found that the calcium ion can be chemically inserted into the crystal structure by using calcium ion solution with a reducing agent. The calcium ion insertion was clearly evidenced by elemental analysis and structure refinement. The electrochemical performance of reversible calcium ion intercalation in a calcium organic electrolyte was also confirmed as well as chemical intercalation, demonstrating the potential as a calcium-ion batteries cathode.

Poster Presentation : **MAT.P-461**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Li-B-S System : Solid Electrolyte for All-Solid-State Battery

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Solid electrolyte is expected to improve stability and performance of Li-ion battery (LIB) by solving the explosion problem of conventional LIBs by replacing separator and organic liquid electrolyte. In this paper, we report the Lithium-Boron-sulfide solid electrolyte (LBSSE) as solid electrolyte candidate for beyond LIBs. The X-ray diffraction data of the synthesized LBSSE show that the material has crystallinity different from the conventional amorphous LBSSE. The electrical conductivity of LBSSE was measured and the conductivity value for Li ion was calculated to be higher than 10^{-5}Scm^{-1} at 300K.

Poster Presentation : **MAT.P-462**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Regenerative Cs ion removal through reversible ion-exchange reaction of alkali metal functionalized graphene oxide fiber

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Recent research works on two dimensional nano-materials offer diverse and promising functionalities within the fields of catalyst, energy storage and conversion, sensor, drug-delivery, and environmental remediation. Among those materials, graphene is a pioneering figure which arise sensation of two-dimensional functional nano-material. In the stream of various graphene oriented research directions, an effort to establish high-yielding and easily dispersible graphene synthesis protocols, graphene oxide is discovered. Graphene oxide, the distinct derivatives of graphene product, can be utilized as a versatile building blocks to yield three-dimensional carbon structure with flexible morphology and functionality. Here we present alkali metal (Na⁺) functionalized graphene oxide (Na-GO) fiber with regenerative radionuclide (e.g. Cs⁺) ion removal functionality. This Na-GO fiber possess high surface area (75-100 m²/g), and broad range of pores (micro-, meso-, and macro), and rapid Cs ion adsorption (132 mg/g) through chemisorption. In addition, once-used fiber can be regenerated with NaOH ion for repeated Cs ion removal. This graphene-oxide fiber offer sustainable remediation functionality through rapid and reversible alkali metal ion-exchange reaction.

Poster Presentation : **MAT.P-463**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Direct Chemical Synthesis of Plasmonic Black Colloidal Gold Superparticles with Broadband Absorption Properties

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Self-assembly of plasmonic metal nanoparticles can provide an opportunity of creating colloidal superparticles with fascinating optical properties arising from interparticle plasmonic coupling, but typically requires multiple steps involving solvent and/or ligand exchange. We developed a direct, one-step chemical synthesis of plasmonic black colloidal Au superparticles with broadband absorption in visible and near-infrared regions. During the synthesis, the Au superparticles were formed through self-assembly of in-situ-formed Au nanoparticles driven by solvophobic interactions between nanoparticles and solvent. These superparticles could be solution-processed to fabricate a thin film, which exhibited near-perfect absorption over a broad range from 400 nm to 2.5 μm as well as the excellent antireflective property. Thanks to their broadband absorption property, the Au superparticles showed good performances for near-infrared surface-enhanced Raman spectroscopy and light-to-heat conversion.

Poster Presentation : **MAT.P-464**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Structure and Electrochemical Characterization of Post-spinel $\text{ZnA}_{0.5}\text{Co}_{1.5}\text{O}_4$ (A = Mn, Ni) as a Cathode Material for Nonaqueous Calcium-ion Batteries

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The rechargeable calcium-ion batteries (CIBs) can be considered as promising alternative of lithium-ion battery systems, being expected to give high performances in terms of the capacity and cost effectiveness due to the relatively much abundance of the calcium. Herein, we investigate the post-spinel structure, $\text{ZnA}_{0.5}\text{Co}_{1.5}\text{O}_4$ (A = Mn, Ni), as a cathode material for nonaqueous CIBs at ambient temperature for the first time. A facile sol-gel method has been applied to synthesize both materials. The Rietveld refinement results from X-ray Diffraction data exhibit a spinel structure with the space group of $Fd-3m$, and the cell parameters of $\text{ZnMn}_{0.5}\text{Co}_{1.5}\text{O}_4$ ($a = b = c = 8.1814 \text{ \AA}$) and $\text{ZnNi}_{0.5}\text{Co}_{1.5}\text{O}_4$ ($a = b = c = 8.0749 \text{ \AA}$), respectively, indicate that Mn and Ni has brought a structural effect. The electrochemical performance was explored by applying Cyclic Voltammetry (CV) test, with activated carbon as counter electrode, and 0.5 M $\text{Ca}(\text{ClO}_4)_2$ in AN as an electrolyte. The CV profiles exhibit small reduction peak appeared at -0.95 V for $\text{ZnMn}_{0.5}\text{Co}_{1.5}\text{O}_4$ and -0.75 V for $\text{ZnNi}_{0.5}\text{Co}_{1.5}\text{O}_4$ versus activated carbon, respectively. Besides, small oxidation peak also appeared at 0.78 V for both samples. However, we believe that the very small reduction and oxidation peaks were due to proton intercalation rather than calcium intercalation, besides further studies are needed to give more evidences.

Poster Presentation : **MAT.P-465**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Spontaneous Deposition of Cobalt Oxide Nanoplates for Application to Acetone Gas Sensors

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The development of sensing materials, which influence the practical gas sensing performance is critically important for the further evolution of semiconducting metal oxide gas sensor. Especially, cobalt oxides have attracted great interest in their potential applications as solid-state sensors because of their chemical stability and semiconducting properties. In this study, we are reporting the spontaneous deposition of Co_3O_4 nanoplates on interdigitated electrodes and its application to gas sensors. Inducing the phase transition of h-CoO to $\text{Co}(\text{OH})_2$ and consecutive thermal oxidation on silicon substrate results in efficient deposition between Co_3O_4 and the substrate without any additional deposition processes. The efficient deposition of Co_3O_4 nanoplates is applicable for acetone gas sensors. Gas-sensing properties of Co_3O_4 nanoplates were investigated using a characterization system with a temperature-controlled hot chuck in a water-cooled steel chamber. The gas response is defined as the ratio of resistance, $R = R_g/R_a$, where R_a and R_g are the resistance in an air and in a gas atmosphere, respectively. The real-time gas response of Co_3O_4 nanoplates were measured under the standard condition with the exposure of 1 ppm acetone gas at 200 °C. The Co_3O_4 nanoplates exhibited quite higher gas sensitivity, and better stability than previous results.

Poster Presentation : **MAT.P-466**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Nanobead-based sensitive immunosensor using amphiphilic functional copolymer

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Korea*

We developed nanobead multilayer-based sensitive immunoassays using amphiphilic functional copolymer. We developed an amphiphilic copolymer comprising benzyl, polyethylene glycol, and reactive ester moieties. Polystyrene nanobeads were reacted with the polymer-coated COC surface and further assembled into multilayers that increased the overall surface area available for attaching capture antibodies. Finally, a sandwich immunoassay was carried out using rabbit IgG as a target analyte and rhodamine-labeled anti-rabbit IgG as a probe. Compared with a nanobead-free, polymer-coated COC surface, the nanobead multilayer-based immunoassay exhibited ~4-fold higher fluorescence intensity. In addition, our nanobead-based assay system exhibited a wide dynamic range of detection (0.1 to 1000 ng/mL) and high specificity for rabbit IgG, indicating the potential value of the proposed immunoassay system in plastic-based portable biochip applications.

Poster Presentation : **MAT.P-467**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Preparation of Porphyrin- POSS (polyhedral oligomeric silsesquioxanes) Nanomaterials and Its Cellular Uptake Studies

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We have prepared the series of porphyrin-POSS (polyhedral oligomeric silsesquioxanes) nanomaterials. Studies on their synthesis, characterization and the cellular uptake properties have been performed. We have studied their spectroscopic properties and cellular uptake properties which depend on the numbers of POSS units and the position of POSS relative to the porphyrin unit. We also have investigated the possibility of porphyrin-POSS nanomaterials as a potential biomaterial for photodynamic therapy.

Poster Presentation : **MAT.P-468**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Interstitial oxygen in the Ga-based Langasite-type oxygen ion conductor: Maximum Entropy Method and Bond Valence Energy Landscape analysis

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A langasite-type $\text{La}_3\text{Ga}_5\text{GeO}_{14}$ has been studied primarily as a piezoelectric material. The crystal structure of $\text{La}_3\text{Ga}_5\text{GeO}_{14}$ is very similar with the melilite, $\text{La}_{1+x}\text{Sr}_{1-x}\text{Ga}_3\text{O}_{7+x/2}$, which has been known to show high oxygen ion conductor. In the melilite structure, lanthanum was equivalently substituted with strontium to add oxygen in the interstitial site, leading to the high oxygen ion conductivity. In this study, we synthesized $\text{La}_3\text{Ga}_{5+x}\text{Ge}_{1-x}\text{O}_{14+x/2}$ ($x = 0 \sim 0.5$) by solid state reaction to introduce interstitial oxygen in the lattice. The crystal structure of $\text{La}_3\text{Ga}_{5+x}\text{Ge}_{1-x}\text{O}_{14+x/2}$ ($x = 0 \sim 0.5$) was characterized by synchrotron powder X-ray diffraction. The $\text{La}_3\text{Ga}_{5+x}\text{Ge}_{1-x}\text{O}_{14+x/2}$ ($x = 0 \sim 0.5$) crystallize hexagonal symmetry with space group $P 321$. The oxygen ion conductivity was measured up to $900^\circ\text{C} (\pm 5)$, the highest ion conductivity was $2.13 \times 10^{-3} \text{ S/cm}$ ($x = 0.4$) and the activation energy was 1.12 eV ($x = 0.4$). The position of interstitial oxygen was confirmed by Maximum Entropy Method (MEM). In order to identify the possible pathways for oxygen diffusion, Bond Valence Energy Landscape (BVEL) maps were calculated.

Poster Presentation : **MAT.P-469**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

New lithium-ion conductors based on the NASICON structure

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Framework oxides based on sodium (Na) super ionic conductor (NASICON) structure are of special interest, because these materials exhibiting high conductivities combined with low activation energies. NASICON structure deserves further attention towards tailoring new lithium-ion conductors for application as electrolytes in solid state lithium batteries. In this study, we synthesized $\text{LiTa}_{1.33}\text{Mg}_{0.66}(\text{PO}_4)_3$ by solid state reaction. The crystal structure was characterized by powder X-ray diffraction. $\text{LiTa}_{1.33}\text{Mg}_{0.66}(\text{PO}_4)_3$ was crystallized rhombohedral symmetry with space group $R\bar{3}c$. In addition, we measured its ionic conductivity and compared with other compounds.

Poster Presentation : **MAT.P-470**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Precisely Shaped, Uniformly Formed Gold Nanocubes with Ultrahigh Reproducibility in Single-Particle Scattering and Surface-Enhanced Raman Scattering

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Synthesizing plasmonic nanostructures in an ultraprecise manner is of paramount importance because the nanometer-scale structural details can significantly affect their plasmonic properties. Au nanocube (AuNCs) have been a highly promising, heavily studied nanostructure with high potential in various fields, but an ultraprecise synthesis from 10 to 100 nm in size over a large number of AuNCs has not been well established. Precisely structured AuNC-based studies for a highly reproducible, quantitative plasmonic signal generation [e.g., quantitative surface-enhanced Raman scattering (SERS)] are needed for reliable use and exploration in the beneficial properties of AuNCs. Here, we developed a strategy for AuNC synthesis with the desired size and shape, ranging from 17 to 78 nm particularly with highly controlled corner sharpness, by precisely controlling the growth rate of different facets and AuNC-specific flocculation which enabled ultrahigh yields (~98–99%). Importantly, the precisely shaped AuNCs can scatter light in a spectrally reproducible manner, and the SERS enhancement factors (EFs) for the AuNC dimers are very narrowly distributed (the EFs of 72 nm sharp-cornered cube dimers have a distribution within 1 order of magnitude). Our results pave the paths to ultrahigh yield synthesis of metal nanocubes with a precise size and shape and offer single-particle-level spectral controllability and reproducibility over a large number of particles.

Poster Presentation : **MAT.P-471**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Study of coating layer control and chromaticity change of α -FeOOH@SiO₂ using basic catalyst

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A hollow metal micro/nanomaterial with a porous structure is one of the most attractive structures for catalysts. Porous silicas have attracted considerable attention because of their distinguished performance in adsorption technology, catalysis, and medical applications. In order to investigate the effect of the density of the silica coating layer on the color of the pigment, we tried to change the structure of the silica layer arbitrarily using a basic catalyst. In this study, we coated SiO₂ on α -FeOOH nanorod and we tried to change the structure of the coating layer using a basic catalyst. We used a basic catalyst to control the structure (pore, density) of the silica layer. The change of shape was observed by TEM analysis and we selected the appropriate reaction time and compared the chromaticity according to the silica layer structure. In particular, it was confirmed that yolk-shell structure of α -FeOOH pigments had a median chromaticity value.

Poster Presentation : **MAT.P-472**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

High-permittivity dielectrics in Nb-based Perovskite Oxynitrides

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Oxynitride-type perovskites BaTaO₂N and SrTaO₂N possess dielectric constants (κ) exceeding 1000, which was attributed to the inherent local distortion and polarizable environment of Ta. Given the chemical resemblance between Ta and Nb, and the general tendency of the latter being more polarizable, it was duly expected that the Nb-analogues would display even higher than the above Ta-oxynitrides. But, the dielectric behaviour of the Nb-perovskite oxynitrides has never been observed so far. We regard that the dielectric polarization in Nb compounds is hindered by the presence of reduced Nb species such as NbN and NbO_xN_y, which can readily occur during the ammonolytic synthesis. To suppress the Nb reduction in the perovskite oxynitride, two different approaches were employed, particularly in the preparation of BaNbO₂N. First, the starting reactants were provided with Ba/Nb > 1, to avoid the possibility of excess Nb. Second, part of Nb was replaced with lower-valent cations, to form BaNb_{1-x}M_xO_{2+4x}N_{1-4x} (M = Li, Na). Diffuse-reflectance spectroscopy and X-ray photoelectron spectroscopy indicated that the introduction of M⁺ is effective in preserving the Nb⁵⁺ state. The κ of BaNb_{0.9}M_{0.1}O_{2.4}N_{0.6} (M = Li, Na) was measured to be >10000.

Poster Presentation : **MAT.P-473**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Precursor-assisted synthesis and electrical property of complex perovskites $\text{La}_3\text{Ni}_2\text{MO}_9$ ($M = \text{Nb}, \text{Ta}$)

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Double perovskites, $\text{La}_3\text{Ni}_2\text{MO}_9$ ($M = \text{Nb}, \text{Ta}$) were prepared by solid-state reaction between NiO and the respective oxide La_3MO_7 . Compared with the conventional route using binary reactants, the present method provides improvements in the phase-purity as well as the synthesis time. Both $\text{La}_3\text{Ni}_2\text{MO}_9$ were crystallized in a monoclinic symmetry ($P2_1/n$), with a rock-salt type complete ordering of Ni and $\text{Ni}_{0.33}\text{Ta}_{0.67}$ on the perovskite B-site. The transport property of $\text{La}_3\text{Ni}_2\text{MO}_9$ was examined by 2-probe impedance spectroscopy using = 80 % dense specimens. The two $\text{La}_3\text{Ni}_2\text{MO}_9$ compounds, without a significant difference depending on the type M , showed Arrhenius-like temperature dependence over 144-420 K, where the conductivity ranged between 10^{-7} to 10^{-2} S/cm with activation energies of = 0.22 eV. It was notable that the present conductivity values are lower than previous literature data by about two orders of magnitude. It is conjectured that the synthesis of $\text{La}_3\text{Ni}_2\text{MO}_9$ can suffer from a compositional deviation to $\text{La}_3\text{Ni}_{2+x}\text{M}_{1-x}\text{O}_9$, in which case, electrical conductivity should be affected by the occurrence of Ni^{3+} .

Poster Presentation : **MAT.P-474**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Crystal Structure Analysis and Dielectric Properties of Tetragonal Tungsten Bronzes, BaTa_2O_6 , $\text{Ba}_{0.8}\text{Ta}_2\text{O}_{5.8}$, and $\text{Ba}_{0.5}\text{Ta}_2\text{O}_{5.5}$

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The Ba-Ta-O ternary system provides an interesting case where the tetragonal tungsten bronze (TTB) phases are formed over a wide compositional range, $\text{Ba}_{1-x}\text{Ta}_2\text{O}_{6-x}$ ($0 \leq x \leq 0.65$). Compared with the most common composition type of the TTB phases, AB_2O_6 , $\text{Ba}_{1-x}\text{Ta}_2\text{O}_{6-x}$ is highly off-stoichiometric and is presumed to involve considerable structural modifications from the regular TTB. In this study, ternary oxides were prepared with the chemical compositions of BaTa_2O_6 , $\text{Ba}_{0.8}\text{Ta}_2\text{O}_{5.8}$, and $\text{Ba}_{0.5}\text{Ta}_2\text{O}_{5.5}$ corresponding to $x = 0$, 0.2, and 0.5, respectively. Rietveld refinement and Fourier electron density calculation, using the high-resolution synchrotron X-ray diffraction data, reveal that the above three composition have distinct local structural features, and the irregularity escalated with the increase of x . In all three cases, the Ba position (A2 site) inside the pentagonal tunnel was slightly scattered, reflecting the oversized polyhedral volume. In $\text{Ba}_{0.8}\text{Ta}_2\text{O}_{5.8}$, the triangular tunnel (A3 site) was partially occupied by Ta. In addition, $\text{Ba}_{0.5}\text{Ta}_2\text{O}_{5.5}$ has segments of $-\text{Ta}-\text{O}-$ chains in the pentagonal tunnel. The dielectric properties of those three samples were measured in the temperature range of 30-450 K, and at 1 kHz, 10 kHz, 100 kHz and 1 MHz.

Poster Presentation : **MAT.P-475**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Bandgap tuning and XPS study of SnO₂ quantum dots

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In the present study, we investigated the influence of annealing temperature on ultra-small SnO₂ quantum dots (SQDs) prepared by a simple chemical reduction process. The structural and optical properties of annealed SQDs were systematically examined by different techniques. Our results show that the crystallinity and average crystallite size of annealed SQDs increased gradually with annealing temperature. The average crystallite size was maintained below 10 nm even for high annealing temperatures. XPS peak fitting analysis yielded information on the presence of mixed ionic states of Sn²⁺ and Sn⁴⁺ in SQDs and further revealed that the number of Sn²⁺ ions decreased at high temperature. Band-edge shifts were estimated from XPS data. It was possible to shift the bandgap of annealed SQDs from UV to the visible wavelength region, which is likely to have a beneficial impact on many applications of optoelectronic devices.

Poster Presentation : **MAT.P-476**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Thermal stability and mechanical properties of organoclay/EVA nanocomposites depending on host clays and organic modifiers

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Nanocomposites of EVA with various organoclays have been prepared by solution blending method, depending on structure of organic modifiers, the content of organoclay and kind of host clay. However, due to the hydrophobicity of EVA polymer, it is usually necessary to modify the hydrophilic surface of clay to hydrophobic one. Therefore we modified the surface of clays such as Kunipia-F (KF), ME-100 (ME), and Laponite (Lap) to be hydrophobic by intercalating the long chain alkylammonium surfactant such as dimethyldistearylammonium bromide (DMDSA) and cetyltrimethylammonium bromide (CTA) with different structure, which were confirmed the expansion of basal spacing from the X-ray diffraction (XRD) analysis. Organoclay/EVA nanocomposites were synthesized by mixing the organoclays dispersed in toluene with EVA dissolved in toluene and evaporating the solvent. According to XRD analysis, the sharp peaks corresponding to the organoclays were diminished in organoclay/EVA nanocomposites, indicating that organoclays were predominantly exfoliated in EVA matrix. The well-dispersed state of organoclay in EVA matrix was also confirmed with the transmission electron microscopic analysis. Thermogravimetric analysis (TGA) show that CTA-clays/EVA nanocomposites have more improved thermal stability than DMDSA-clays/ EVA. In case of CTA-ME/EVA and CTA-KF/EVA, the decomposition temperature of EVA was proportionally improved by 25 °C compared to pure. The mechanical properties was also performed with the different organoclays content (1-12 wt%). The elastic modulus and tensile strength of nanocomposites gradually increase with the higher loading of clay filler, and this enhancement also can be seen indicated the larger compatibility between EVA matrix and layer silicates.

Poster Presentation : **MAT.P-477**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Graphitic Carbon Nitride-Clay Nanohybrid as A New UV shielding Material

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Graphitic carbon nitride (g-C₃N₄) has received a great attention not only due to its unusually high chemical and thermal stability, but also its various physico-chemical functions applicable for visible light harvesting photocatalyst, metal-free catalyst, reactive template and nitrogen source of nitridation reaction. In this study, we developed a novel soft chemical route to g-C₃N₄ nanosheets confined in 2D nanoreactor (Mica) by intercalating cyanamide, a precursor of g-C₃N₄, into layered mica and its subsequent pyrolysis. In brief, cyanamide was first intercalated into mica via solid state reaction at 100°C for 3 hrs to form cyanamide-mica nanohybrid. The cyanamide in the interlayer space of mica was polymerized to g-C₃N₄ at 550°C for 4hrs. According to the X-ray diffraction (XRD) and transmission electron microscope (TEM) analyses, the basal spacing of mica (0.96 nm) was expanded to 1.50 nm for cyanamide-mica and 1.28 nm for g-C₃N₄-mica nanohybrids, respectively, indicating that cyanamide was successfully intercalated into interlayer space of mica and polymerized to g-C₃N₄ with single supramolecular structure. The intergallery height of g-C₃N₄-mica nanohybrid was determined to be 0.32 nm which is exactly the same as the single atomic layer thickness of graphite indicating the formation of single sheet g-C₃N₄. The g-C₃N₄-mica nanohybrids as well as bulk g-C₃N₄ showed excellent UV absorption properties below 450 nm. However, the photocatalytic activity of g-C₃N₄-mica hybrid was almost quenched, due to the effective screening of photoactive site by insulating mica. It is, therefore, concluded that the present g-C₃N₄-mica could be applicable as the UV-screening agent due to its excellent UVA-UNB-UVC (200~400 nm) screening property without any photocatalytic degradation and phototoxicity.

Poster Presentation : **MAT.P-478**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

InP nanorod/rGO/FTO glass for CO₂ to CH₃OH conversion

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Ongoing research of the carbon capture and utilization (CCU) became important challenge since the storage of captured carbon technique for CO₂ reduction resulted in re-emission. There are several CO₂ conversion processes such as a thermal reduction with catalyst, electro-catalytic reduction, biochemical reduction and photocatalytic reduction. Especially photocatalytic CO₂ reduction process is analogue to solar water splitting. That is, photocatalysts that were applied for hydrogen evolution could be also used for CO₂ reduction. In this study, InP was vertically grown on FTO glass by chemical deposition for visible light absorption and selectivity of methanol synthesis. rGO was synthesized by improved Hummer's method. Microstructures were confirmed by means of both FESEM (field emission scanning electron microscope) and TEM (transmission electron microscope). Its anisotropic growth mechanism was proposed that dissolution and specific precipitation. CO₂ to CH₃OH conversion test was conducted using three electrode system under visible light that of intensity 100mW/cm². Products of CO₂ reduction was collected by micro-syringe and subsequently transferred to the quartz cuvette involving chemical reagent of CH₃OH to coloured solution conversion selectively for qualitative measurement by UV-Vis absorbance. Quantitative measurement of CH₃OH was also conducted by GC-MS (gas chromatography-mass spectrometer).

Poster Presentation : **MAT.P-479**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

g-C₃N₄/TiO₂ NPs Impregnated Polyethylene Composite Media for Hydroponics

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Hydroponics is a method to grow plants without soil. This method has been attention to produce foods for future against a gradually increasing serious contamination of soil, a drought, damages from insects and a climate changing. In addition to it has several controllable properties such as a growing period, composition of nutrients, high additive plants production, CO₂ reduction and saving water. In order to cultivate plants using hydroponic method, media as standing seeds and absorbing nutrient solution, green, red, blue and white LED for photosynthesis, temperature and humidity control system, circulating nutrient and recycling system and suitable CO₂ atmosphere for photosynthesis are required. Among these requirements, media materials dominantly determine successful growing plants because it acts nutrient and water container to supply with balance. Rock wool as popular medium is a molten mineral came from volcano over 1600 °C. However it causes environmental contamination because it is hardly degradable and high temperature melting process is required. Recently alternative media has been studied such as rice husk, coconut based media and fishbone. But theses eco-friendly media have low nutrient and water contents as well as biological contamination that decrease media performance. Therefore now new media materials involving similar properties of rock wool but easier degradation without contamination are needed. In this work, biodegradable microporous polyethylene with g-C₃N₄/TiO₂ NPs composite are suggested as an alternative of rock wool. Microporous polyethylene was prepared phase inversion method. g-C₃N₄ and TiO₂ nanoparticles were prepared by sol-gel and hydrothermal method. Hydroponic test equipment was consisted of transparent plastic, LED, air supply, CO₂ gas control system, PVC media bed circulation system of nutrient solution with pump and temperature/humidity controller. Properties of media were compared with present rock wool and coconut based media by growing plants. Organic-inorganic composite media show better growing control than present media such as growth of root, shape of leaf and length.

Poster Presentation : **MAT.P-480**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Decomposition of CH₄ gas using TiO₂ Nanotubes/Optical Fibers for Trace Contaminant Control System of Spacecraft

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Decomposition of volatile organic compounds (VOCs) by means of photocatalysts has been studied for designing of spacecraft and spacesuit. Especially for long period mission such as planet exploration, because they cause diseases such as central nervous disorder, irritation of mucosa and arrhythmia. As present VOCs control system that are composed by a charcoal bed for adsorption, a sorbent bed(2kg of LiOH/day-person, LiOH affects irritation of eyes) and a catalytic oxidizer(operated at 400°C) is heavy, high power consumption and complex, thus, newly development of compact, efficient and highly durable VOCs control system is required now. In this study, we suggested that TiO₂ nanotubes enable to reduce weight of present VOCs control system and hazardous LiOH replacement. What we suggest that TiO₂ nanotubes mean having wide band gap is to be enable effective charge separation and catalysis. TiO₂ is not available at visible-light irradiation due to its wide band gap of 3.2eV. Thus, QDs as visible light absorber deposited TiO₂ nanotubes were prepared by chemical bath deposition in convection oven. TiO₂ nanotubes were characterized for decomposition of VOCs that confined on surface of tube walls to protect astronauts against VOCs. VOCs for decomposition test were considered based on spacecraft maximum allowable concentrations table from NASA. Their efficiency of VOCs decomposition in both TiO₂ nanotube-coated optical fibers will be investigated and evaluated in the trace contaminant system of spacecrafts.

Poster Presentation : **MAT.P-481**

Material Chemistry

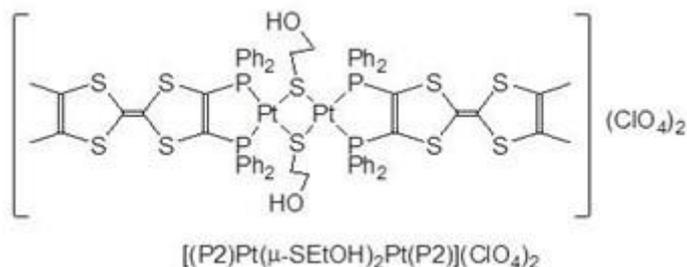
Grand Ballroom, THU 11:00~12:30

MALDI-TOF mass spectroscopic investigation on the rearrangement of [(P-P)Pt(μ -SEtOH)₂Pt(P'-P')](ClO₄)₂ complexes

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Heteroleptic di-Pt(II) complexes formulated as [(P-P)Pt(μ -SEtOH)₂Pt(P'-P')](ClO₄)₂ where P-P and/or P'-P' are dppe (1,2-bis(diphenylphosphino)ethane), dpfp (1,1'-bis(diphenylphosphino)ferrocene) and **P2** (bis(diphenylphosphino)dimethyltetrafulvalene), are prepared by combination reaction of (P-P)Pt(SEtOH)₂ and (P'-P')Pt(ClO₄)₂. The fragmentation and re-organization of mono-Pt(II) and di-Pt(II) complexes are investigated by MALDI-TOF MS. Consequently, it is verified that (P-P)Pt(SEtOH)₂ is re-organized to the corresponding di-Pt(II) complex. Moreover, [(P-P)Pt(μ -SEtOH)₂Pt(P'-P')]²⁺ ions are fragmented to [(P-P)Pt(μ -SEtOH)]⁺ and [(P'-P')Pt(μ -SEtOH)]⁺ ions, and re-organized to [(P-P)Pt(μ -S)(μ -SEtOH)Pt(P'-P')]⁺, [(P-P)Pt(μ -S)(μ -SEtOH)Pt(P-P)]⁺, and [(P'-P')Pt(μ -S)(μ -SEtOH)Pt(P'-P')]⁺ ions. The mass peaks for these fragments are confirmed by fitting with theoretical values. The fragmentation and re-organization processes are suggested on the basis of MALDI-TOF MS results. This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF2010-0011478).



Poster Presentation : **MAT.P-482**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Biocompatible Nanohybrid Fiber Formation of Polyvinyl alcohol (PVA)/ Poly(acrylic acid) (PAA)/ Layered double hydroxides under Various Electrospinning Conditions

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At first, the formation of nanofibers with poly(vinyl alcohol) (PVA)/layered double hydroxide (ZnAl LDH, ZnCuAl LDH) composites were examined by electrospinning method with an applied potential of 19 kV. Either inorganic colloidal LDH (C-LDH) or powder LDH (P-LDH) was used for incorporating with PVA in an aqueous solution. Scanning electron microscopy (SEM) images for thus prepared fibers suggested that C-LDHs were better dispersed than P-LDH within PVA matrix without forming any aggregates, but with a small content of beadings formation. This is surely due to the fact that P-LDH nanoparticles were not dispersed completely and eventually conglomerated in the PVA matrix. In the present study, therefore, all the PVA/C-LDH fibers were further developed by adding poly(acrylic acid) (PAA) solution in order to enhance the chemical interaction between LDH and polymers, and by changing the synthetic parameter like the content of C-LDH in order to escape from the formation of beadings. Since PAA is a hydrophilic polymer, it can easily be incorporated with PVA one to form hybrid fibers due to an enhancement of hydrogen bonding interaction between them and also with LDH, as well. As expected, PVA/PAA/C-LDH fibers were well prepared without forming any aggregates and beadings, due to an enhanced dispersion of LDH nanoparticles in the PVA/PAA matrix and as a consequence, its electrospinnability was improved. The cytotoxicity of PVA/PAA/C-LDH (ZnAl LDH, ZnCuAl LDH) nanofibers was evaluated on the basis of an indirect cytotoxicity assay after the cells were cultured with the extracted media from nanofibers for 48h. PVA/PAA/C-ZnAl LDH nanofibers showed more than 80 % cell viability enough to be used as non-toxic and biocompatible materials.

Poster Presentation : **MAT.P-483**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Paracellular Transport Behavior of Negatively Charged 2D Nanoparticles Based on In-Vitro Follicle Associated Epithelial Model

Jiyeong Kim, Goeun Choi¹, Jin-ho Choy^{1,*}

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¹Department of Chemistry and NanoScience, Ewha Womans University, Korea

Oral drug delivery is the most common route for drug administration due to its safety and convenience. One of various oral drug delivery vehicles, anionic clay, such as layered double hydroxides (LDHs), has been attracted a great deal of attention due to its high biocompatibility, high drug loading capacity and controlled release property. In this study, in-vitro human Follicle-associated epithelium (FAE) model was used to understand the transport pathways of 2D nanoparticles with respect to their particle sizes from 100nm to a few μm , how they could be translocated across the cellular monolayer. A decrease in transepithelial electrical resistance (TEER) for the Caco-2 and Raji B co-cultured monolayers incubated with LDH nanoparticles indicated that the paracellular tight junctions became loosened. We also found that the paracellular transport of nanoparticles was size-dependent, and that the 100nm sized LDH showed better translocation than the other sized. It is, therefore, concluded that the present 2D nanoparticles were translocated through paracellular transport pathway as well confirmed by the confocal images of co-culture cell monolayer.

Poster Presentation : **MAT.P-484**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

Tuning mesopores of carbon electrodes for boosting capacitance of electrochemical energy storage

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¹Department of Chemical and Molecular Engineering, Hanyang University, Korea

Electrochemical double layer capacitors (EDLCs) store electrochemical energy via adsorbing electrolyte ions on the electrode surface; thus high surface area and electrical conductivity are necessary. Therefore, there are tremendous efforts to increase the surface areas, mainly achieved from development of micropores and small mesopores, and electrical conductivity via incorporation of nitrogen atom for high performance of EDLCs. There have, however, been less focused on the effect of relatively large mesopores (> 10 nm) for capacitance of EDLCs. In this poster, we synthesized 3-dimensionally ordered mesoporous carbons (3DOMCs) by hard template method through infiltration the carbon precursor into the silica templates (20-50 nm). Capacitances of EDLCs of the different sizes of mesopores (20, 40, and 50 nm) of 3DOMCs with similar surface areas were investigated and the correlation between the size of mesopores and capacitances will be presented. In addition, in order to more boost the capacitance, CO₂-activation process was applied to develop surface area of 3DOMCs.

Poster Presentation : **MAT.P-485**

Material Chemistry

Grand Ballroom, THU 11:00~12:30

A Novel Geopolymer Route to Microporous Carbons with Effective CO₂ Uptake Capacity

Yirong Pei, Goeun Choi, Jin-ho Choy*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

A novel geopolymer route to microporous carbons with high specific surface area and large pore volume was reported in this research. The present low-cost process is composed of 2 steps; (1) synthesis of porous geopolymer (PG) from metakaolin, which can be prepared by heating natural kaolin up to 700 °C and (2) synthesis of porous carbons (CPG) replicating from PG with the carbon source such as sucrose and gelatin, respectively. The porous nature of PG was observed to be mesoporous with a pore diameter of 2.90 nm and a well-ordered hexagonal channel structure. The porous CPG-S replicated from this PG template with sucrose was determined to be highly microporous with the BET surface area of ~ 1200 m²/g and the pore volume of ~ 1.2 cm³/g, but with the small amount of meso and macropores. According to the CO₂ uptake experiments for the present CPG-S, the high capacity of 3.08 mmol/g could be observed even at 273 K and 1 atm due to the physi-sorption of CO₂. In case of CPG-G, which was replicated with the gelatin carbon source, it exhibited relatively high uptake capacity under relatively lower pressure (< 0.10 atm) owing to the chemi-sorption of acidic CO₂ on Lewis basic N-functionalized internal surface. When the mixed carbon precursor of sucrose and gelatin (1:1 mass ratio) was used, a synergistic effect could be observed in terms of porosity and N-functioned internal surface as well demonstrated with the highest CO₂ uptake capacity under the pressure range of 0.20 ~ 0.65 atm. It is, therefore, concluded that the present geopolymer template route to microporous carbons could offer an effective and low-cost strategy and eventually provide a promising way of industrial applications of porous carbons.

Poster Presentation : **ELEC.P-457**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Activating MoS₂ basal plane with Ni₂P nanoparticles for hydrogen evolution reaction in acidic media

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¹*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

The hydrogen production via electrochemical water splitting is a sustainable way to address both energy and environmental issues of the world. An efficient, durable and cheaper electrocatalyst is desired for effectively catalyzing hydrogen evolution reaction (HER) in real applications. The noble metals (Pt, Ru) based are most efficient catalysts in acidic electrolyte due to their low metal-hydrogen (M-H) bond strength desired for fast HER kinetics. Two dimensional MoS₂ is considered as an alternative Pt that displays a modest hydrogen evolution reaction (HER) activity in acidic media because the active sites are limited to a small number of edge sites with broader basal planes remaining mostly inert. Here we report that the basal planes could be activated by growing Ni₂P nanoparticles on it. Thus, a Ni₂P/MoS₂ heterostructure is constructed via in-situ phosphidation of an ingeniously synthesized NiMoS₄ salt to form a widely cross-doped and chemically connected heterostructure. The conductivity and stability of the Ni₂P/MoS₂ are further enhanced by hybridization with conductive N-doped carbon support. As a result, the Ni₂P/MoS₂/N:RGO or N:CNT displays Pt-like HER performance in acidic media, outperforming the incumbent best HER electrocatalyst, Pt/C, in more meaningful high current density region (>200 mA/cm²) making them a promising candidate for practical water electrolysis applications. Non-precious metal catalysts showing Pt-like HER performance in acidic media are rare, our hybrid catalyst is a promising candidate for practical hydrogen production via water electrolysis.

Poster Presentation : **ELEC.P-458**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Efficient electrocatalysis to water dissociation via chemical strain formation through anion substitution in ternary transition metal chalcogenides

Anand prakash Tiwari

Material science and engineering, Korea Advanced Institute of Science and Technology, Korea

To date, researchers have revealed that the electrocatalytic activity can be improved by the creation of defects in the crystal lattice of 2-dimensional layered, transition metal chalcogenides (TMCs) such as MoS₂ or Cu₂MoS₄, respectively. However, the role of anion substitution for the enhancement of overall electrocatalytic activity in the ternary TMCs (TTMC) remains unproven. Here, we show the substitution of anion atom sulfur (S) with selenium (Se) in a new electrocatalyst Cu₂WS₄ for efficient hydrogen evolution reaction (HER) activity. The higher electrocatalytic activity of Cu₂WS₄ after anion atom substitution can be attributed to the creation of chemical strain in the lattice, which causes an increase of active sites for hydrogen adsorption and desorption. Experimentally, the anion substituted Cu₂W(S_ySe_{1-y})₄ sample shows superior electrocatalytic activities with low onset potential of 0.320 V at 10 mA/cm² for HER, which is two-fold lower than the pristine Cu₂WS₄ (0.650 V at 10 mA/cm²) sample. In addition, after 1,000 cycles with continuous electrolysis in an acid electrolyte for 12 h, the anion substituted samples Cu₂W(S_ySe_{1-y})₄ preserves its structure and robust catalytic activity perfectly. As a result, our work demonstrates a new approach for the developments of real applications of TMCs in energy conversion.

Poster Presentation : **ELEC.P-459**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

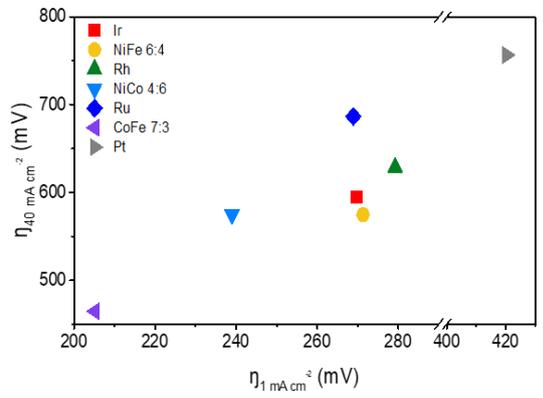
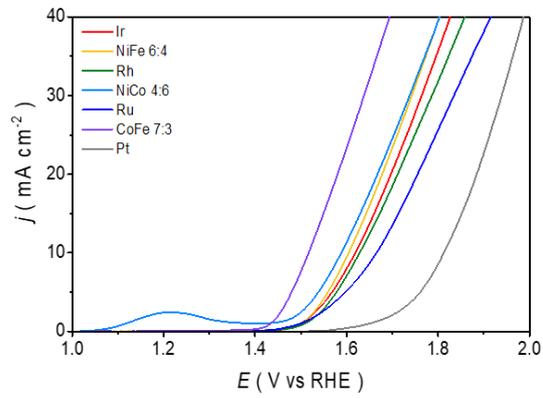
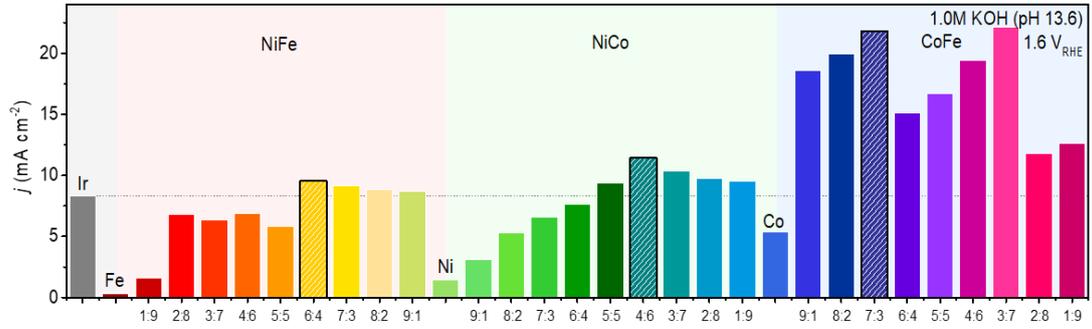
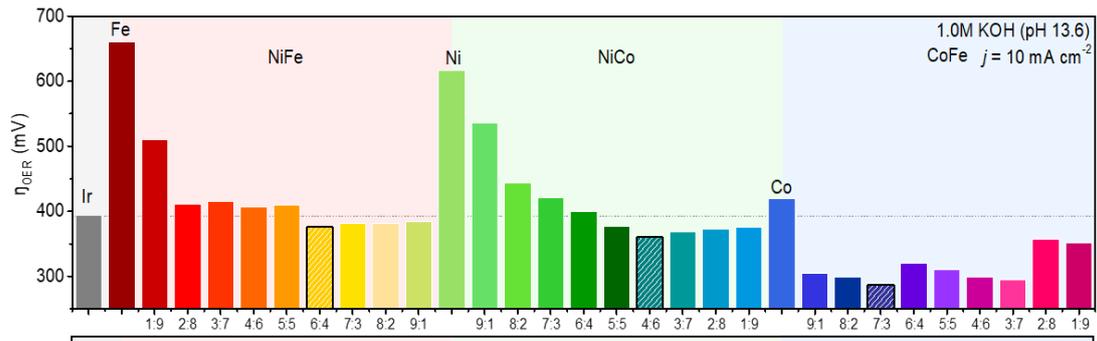
Amorphous metal oxide containing Iron, Cobalt and Nickel by precipitational route for oxygen evolution catalysts and their activity descriptor

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PV-electrolysis of water is an effective route that can transform intermittent renewable energy into a storable chemical fuels such as hydrogen and oxygen. The oxygen evolution reaction (OER) is the most energy consuming step in water electrolysis due to its sluggish four-electron process. Therefore, catalyst is required to lower the kinetic barriers of OER. Catalysts based on Noble metals are known as best oxygen evolution catalyst (OEC) but have low reserve and expensive. As a result, earth abundant transition metal catalysts with reasonable price, high activity and stability have been extensively studied. Most of these catalysts are crystalline metal oxide, but recently catalysts with amorphous properties also show good activity. however, amorphous catalysts exhibit complex synthetic methods, making it hard to amend mixed compositions and descriptors elucidating the tendency of electrochemical activity is absent. Here we develop facile one step precipitational metal nitrate deposition (PMND) method which can modulate mixed metal composition easily on various substrates. The catalysts synthesized by this method have single or various composition of binary metal (oxy)hydroxides structures exhibiting comparable activity with novel metal and high stability in alkaline medium. Characterization of the catalyst using X-ray photoelectron spectroscopy reveals that the tendency of electrochemical activity of OEC depend on the ratio of oxide and hydroxide on the catalyst surface. In this study, a new type of volcano plot was formed by combining the percentage of hydroxide on the catalyst surface with the Tafel slope. This is a new descriptor that can explain the tendency of the catalyst through a broad range of active scans.



Poster Presentation : **ELEC.P-460**

Electrochemistry

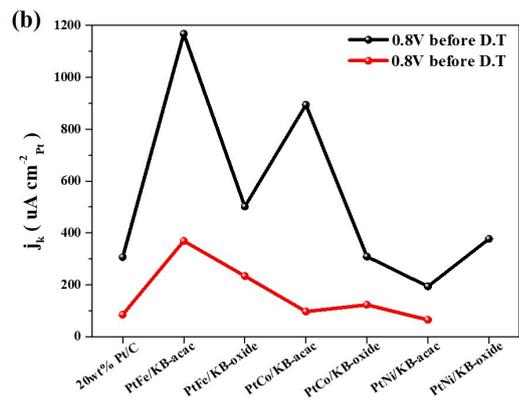
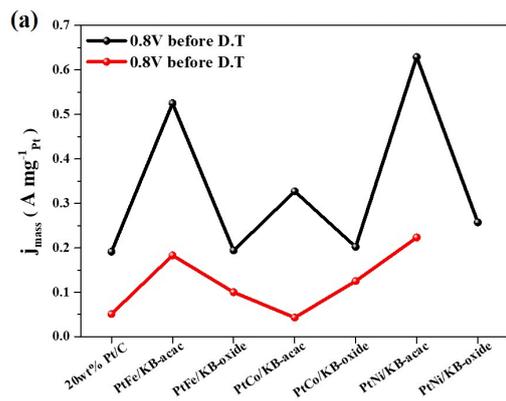
Grand Ballroom, FRI 11:00~12:30

One-pot sonochemical synthesis of Pt-M/C(M=Fe, Co, Ni) Nanoparticles from PtO₂ precursor as durable electrocatalysts for Oxygen Reduction Reaction

Ah-Hyeon Park, Young-Uk Kwon*, Hyun-Uk Park, Wenjuan Shi

Department of Chemistry, Sungkyunkwan University, Korea

Herein, we present Pt-M/C(M=Fe, Co, Ni) nanoparticle with PtO₂ and Pt(acac)₂ precursor for oxygen reduction reaction(ORR) in acidic media and compare their mechanistic difference in synthesis process and catalytic performance caused by it. It was synthesized with sonochemical method that is simple one-step reaction and it is useful to control the metal composition. In structural study, their particle size is 2-3 nm and well-dispersed on carbon support and EDS line mapping data underpin that they synthesize core-shell nanoparticle. In case of PtO₂ precursor, Pt-Ni also synthesized well compare with Pt(acac)₂ precursor and they make oval shape nanoparticle in all case of transition metal unlike Pt(acac)₂ case that make sphere shape particle. Compared their activity, sample synthesized with Pt(acac)₂ show better activity than PtO₂ and both of that better than that of commercial Pt/C. In durability test, sample with PtO₂ better than that of Pt(acac)₂. In sonochemical method, difference of Pt precursor guides different mechanism to synthesize nanoparticle from precursor. We propose that Pt(acac)₂ exist ion form in solution when before Pt reduce from precursor to metal and it can be occurring gavalnic replacement with Fe. While PtO₂ can't be dissolved because it is ionic compound, therefore it makes aggregated Pt particle that is the reason why it is hard to replacement with Fe.



Poster Presentation : **ELEC.P-461**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Hollow manganese oxides nanotube as a bifunctional catalyst for oxygen reduction and oxygen evolution reactions

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Department of Chemistry, Daegu University, Korea

Various transition metal oxides have been widely studied as electrode materials for these reactions because of their wide applications in different fields such as rechargeable batteries, chemical sensing devices, catalysis, and microelectronics. Among transition metal oxides, manganese oxide is one of the most attractive electrode materials for fuel cells and water splitting with environmental friendliness, low cost, and natural abundance. However, its potential application in these fields is limited by its poor electrical conductivity and large volume expansion during repeated cycling processes. In this presentation, we present a simple chemical approach to the synthesis of hollow manganese oxides nanotubes using carbon nanotubes (CNTs) as an efficient template. Manganese oxide produced by the reaction between potassium permanganate and acid is coated on CNT and heat treatment is performed to obtain hollow nanotubes. Such a nanostructure can be used as an electrode catalyst for improved catalytic activity in an oxygen reduction reaction (ORR) and an oxygen evolution reaction (OER). Compositional and structural features are characterized by scanning electron microscopy equipped with an energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The electrocatalytic activity of the manganese oxide nanotubes for ORR and OER in alkaline media was investigated by rotating disk electrode, rotating-ring disk electrode, and cyclic voltammetry. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Poster Presentation : **ELEC.P-462**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Designing Hierarchical Assembly of Carbon-Coated TiO₂ Nanocrystals and Unraveling the Role of TiO₂/Carbon Interface in Lithium-Ion Storage in TiO₂

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Owing to its high chemical stability, structural robustness, abundance, and high working voltage (~1.75 V vs. Li⁺/Li), anatase titanium dioxide (TiO₂) has extensively been investigated as an anode material for lithium-ion batteries (LIBs). In addition, the hierarchical nanostructures of oxide-based electrode materials whose benefits are large surface area, synergistic interactions and high performance have been developed for LIBs. Despite the many benefits of hierarchical nanostructures of oxide-based electrode materials for LIBs, it remains a challenging task to fully exploit the advantages of such materials partly because of their intrinsically poor electrical conductivities. The resulting that limited electron supply to primary particles inside secondary microparticles gives rise to significant variation in lithium-ion (Li⁺) storage capability within the nanostructured particles. To address this, facile annealing, where in situ generated carbon-coated primary particles were assembled into porous microagglomerates, is demonstrated to prepare nanostructured TiO₂. A systematic study on the effect of the carbon coating reveals that it is exclusively governed by the characteristics of the TiO₂/carbon interface rather than by the nature of the carbon coating. This new insight serves as a stepping stone toward understanding an important, yet often overlooked effect of the oxide/carbon interface on Li⁺ storage kinetics, thereby demanding more investigation to establish a new design principle for carbon-coated oxide electrode materials.

Poster Presentation : **ELEC.P-463**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Comparative Study of the effects of Au nanostructures on the electrochemical detection of Arsenic

Camerun Kastro Kanido

Department of Chemistry, Chungbuk National University, Korea

Arsenic is a highly toxic chemical element naturally exists in the form of inorganic and an organic compound which is incorporated in the groundwater and soil. Nanostructure modified gold electrodes play a significant role in sensing inorganic arsenic. In this work, we present the effect of various nanostructures: nanoplate gold, dendritic gold and nanospike gold electrodes in detecting low level of arsenic by using Square Wave Anodic Stripping Voltammetry (SWASV) and the relationships of crystallographic orientations with the performance of the modified electrodes under different experimental parameters: deposition charge, deposition potential and deposition time. The sensitivities of each electrode compared to each other and also further comparison made with flat macro-gold electrodes responses. Investigated that nanoplate gold electrodes show higher performance than dendritic Au, nanospike Au as well as flat gold electrodes. The sensitivities were dependent on the surface crystal orientations which is achieved with the maximum Au(111) facets in nanoplate gold electrodes as confirmed by the Pb UPD voltammetric profile of 0.1M NaOH + 10⁻³ M Pb(NO₃)₂. The higher sensitivity of 127.1 $\mu\text{A } \mu\text{M}^{-1} \text{ cm}^{-2}$ obtained in nanoplate Au electrode at a deposition time of 300s. The interference test conducted in the presence of Cu(II) indicate that nanostructured modified gold electrode detect arsenic(III) successfully in the presence of copper interference.

Poster Presentation : **ELEC.P-464**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

As(III) Detection at Nanoporous Gold Electrode by Square Wave Voltammetry

Min Ji Seo, Camerun Kastro Kanido, Jongwon Kim*

Department of Chemistry, Chungbuk National University, Korea

Nanoporous gold (NPG) has a much larger surface area than the flat gold electrode and is widely used because of its unique physical and chemical properties. In this experiment, when the As (III) detection was performed, it was observed how the electrochemical behavior and sensitivity at NPG electrode were enhanced compared to the flat gold electrode. Furthermore, it was observed how the electrochemical behavior and sensitivity of the As (III) detection changes when the surface area of the NPG electrode is controlled. NPG electrode was prepared by anodization of Au rod surfaces. The surface areas of NPG electrodes were controlled by adjusting the anodizing reaction time. Arsenic (III) detection was carried out by using a square wave voltammetry (SWV) technique at an NPG electrode, and the electrochemical behavior was observed by varying the deposition time and deposition potential to find the optimum condition. Under the optimized experimental conditions, observation of the electrochemical behavior of the Arsenic (III) peak at the NPG electrode showed that the peak was negatively shifted and had greater sensitivity than the flat gold electrode. NPG electrode shows excellent selectivity and anti-interference characteristics against Cu (II) ions. This suggests that the NPG electrode with a large surface area and high sensitivity could be used as a very useful electrode sensor for the detection of Arsenic (III) by square wave voltammetry (SWV).

Poster Presentation : **ELEC.P-465**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Oxygen Evolution Reaction on Nanoporous Gold Modified with Ir and Pt: Synergistic Electrocatalysis between Structure and Composition

Yumi Wang, Jongwon Kim*

Department of Chemistry, Chungbuk National University, Korea

Oxygen evolution reaction (OER) is used in electrochemical devices that store the energy of electricity or light as chemical energy. At this time, there is a problem that OER requires high overpotential because the reaction is more sluggish than hydrogen evolution reaction (HER). Therefore, researching on OER has been investigated to reduce its overpotential. In this study, we used a very large surface area NPG. NPG is applied in many studies because the structure is electrochemically stable and exhibits high catalytic activity in a variety of reactions. However, no significant OER activity was observed with NPG itself. In this study, the NPG surfaces were modified with Pt using atomic layer electrodeposition methods, and the resulting NPG@Pt exhibited enhanced OER activities compared to the NPG and flat Pt electrode. Ir-modified NPG (NPG@Pt) electrodes were prepared by spontaneous replacement of Ir on NPG surfaces, which exhibited enhanced OER activity compared to the flat Ir surfaces. The modification of Ir on NPG@Pt resulted in the NPG@Pt/Ir electrodes, and their OER activity exceeded that of NPG@Ir surfaces. As a result, the OER activity on NPG@Pt/Ir surfaces demonstrates the synergistic electrocatalysis between structure of nanoporous surfaces and the active OER components. The OER activity was compared using these electrodes and the durability was confirmed by the chronopotentiometry.

Poster Presentation : **ELEC.P-466**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Single water droplet electrolysis and detection using electrochemical collision event in organic solution

Jungeun Lee, Byung-Kwon Kim*

Department of Chemistry, Sookmyung Women's University, Korea

The electrochemical collision method has been universal because of its convenience and feasibility. Herein, we studied the electrochemical oxidation of water in single attoliter water droplet using the emulsion droplet reactor (EDR) technique on an ultramicroelectrode (UME). Current spikes of collision signal were observed in the chronoamperometry, indicating that the electrolysis of single emulsion droplet occurred when a droplet collided to the UME surface. From the collision results, the collision frequency, size distribution and i - t decay behavior of water in oil (W/O) emulsion droplet were obtained.

Poster Presentation : **ELEC.P-467**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical and Optical Characteristics of Water Soluble Phosphate-Functionalized Naphthalene- and Perylene-Diimide and Its Zirconium Bisphosphate Multilayer Films

Yeong Il Kim^{*}, Hyun-Kwan Shim^{*}

Department of Chemistry, Pukyong National University, Korea

The electrochemical and optical properties of phosphate-functionalized naphthalene and perylene diimides, that are N,N'-bis(ethylhydrogen phosphate)-1,4,5,8-naphthalene bis(dicarboximide) (EPNDI) and N,N'-bis(ethylhydrogen phosphate)-3,4,9,10-perylene bis(dicarboximide) (EPPDI), were investigated in aqueous solutions and thin films. The thin films of these materials were prepared layer-by-layer on ITO substrate by the alternate coordination with zirconium ion and the functionalized phosphate. EPNDI could exist as monomeric form in aqueous solution regardless of solution pH, while EPPDI was in dimeric or polymeric form and dependent on pH. The redox properties of both EPNDI and EPPDI were strongly dependent on pH of the electrolyte solution whether they are in solution or thin films on ITO. The electron transfers between EPNDI/EPPDI and ITO electrode were catalyzed by proton. The mediated electron transfer of EPNDI/EPPDI thin films into a redox couple in solution were also investigated.

Poster Presentation : **ELEC.P-468**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Observing phase transition of a temperature-responsive polymer using electrochemical collisions on an ultramicroelectrode

Kim Hae-Young, Byung-Kwon Kim^{1,*}

Sookmyung Women's University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Herein, a study on a new lower critical solution temperature (LCST) polymer in an organic solvent by an electrochemical technique has been reported. The phase transition behavior of poly(arylene ether sulfone) (PAES) was examined on 1,2-dimethoxyethane (DME). At a temperature above the LCST point, polymer molecules aggregate to create polymer droplets. These droplets subsequently collide with an ultramicroelectrode (UME), resulting in a new form of staircase current decrease. The experimental collision frequency and collision signal were analyzed in relation to the concentration of the polymer. In addition, the degree of polymer aggregation associated with temperature change was also observed.

Poster Presentation : **ELEC.P-469**

Electrochemistry

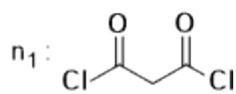
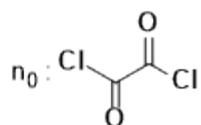
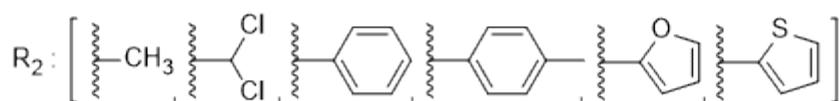
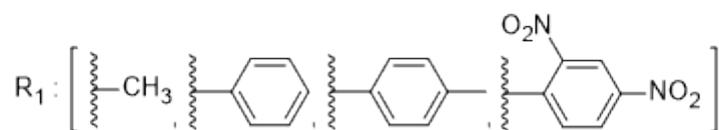
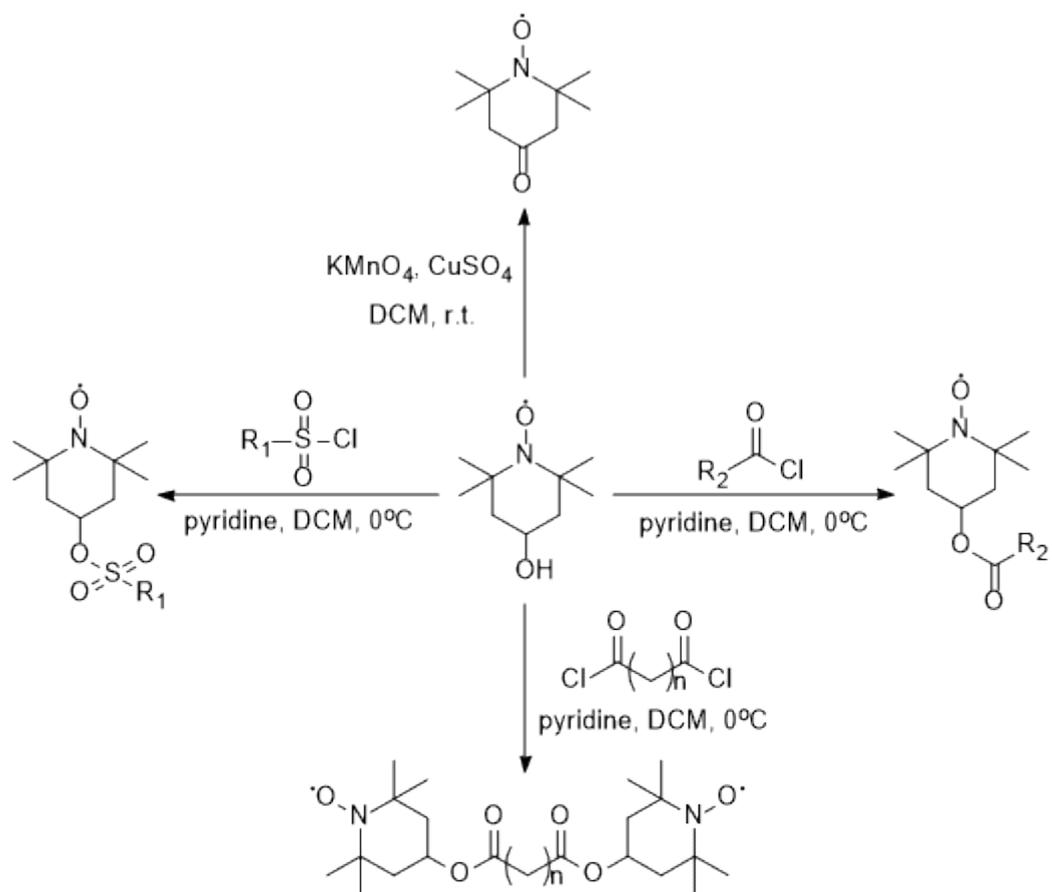
Grand Ballroom, FRI 11:00~12:30

Preparation and Electrochemical Investigation of TEMPOL Derivatives : Apply to Redox Flow Battery

Hyunil Cho, Chujin Ahn*

Department of Biology and Chemistry, Changwon National University, Korea

Recently TEMPOL derivatives are known the possibility of wide potential windows for Redox Flow Batteries(RFBs) as organic catholyte. Herein we report the investigation on electrochemical properties of TEMPOL derivatives. To do this we prepared TEMPOL derivatives and investigated CV results depending on their different functional group. Also the best result of TEMPOL derivatives was applied to RFBs system and measured the VRFBs cell efficiency with TEMPOL Acetate derivative.



Poster Presentation : **ELEC.P-470**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrocatalytic CO₂ Conversion to CO on Gold Nanoclusters in a Flow Electrolyzer

Hoeun Seong, Yongjin Lee, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Electrochemical reduction of CO₂ is a promising technology to mitigate CO₂ emissions and store intermittent renewable energy. Among the electrocatalysts for CO₂ reduction, Au based materials are reported to show the highest activity and selectivity, but polycrystalline Au electrodes still suffer from discontinued selectivity, catalytic rates, and rather high overpotential. In this poster, we present that atomically precise ligand protected gold nanoclusters, such as Au₂₅(SR)₁₈, where SR is thiolate ligand, can effectively and selectively convert CO₂ to CO. The CO₂ electroreduction was studied with Au₂₅(SR)₁₈ nanoclusters immobilized on carbon-based gas diffusion electrode under various pH conditions in a flow electrolyzer. We found that Au₂₅(SR)₁₈ nanoclusters can convert CO₂ to CO with high selectivity (>90%) with high current density over 300mA cm⁻² under 3M KOH. In terms of cell potential, we achieve ~1.6V of cell onset potential ($|\eta_{\text{cell}}| = \sim 0.3\text{V}$), with Au₂₅ nanoclusters as cathode catalysts and IrO₂ as anode catalysts. Additionally, we found that electrolyte plays a key role in catalytic activity of Au nanoclusters. Electrocatalytic rates of Au nanoclusters were higher under KOH solution rather than under KCl solution that has same molarity. Moreover, with increase of KOH concentration, higher j_{CO} (CO partial current densities) values are observed, maintaining selectivity for CO over 90%.

Poster Presentation : ELEC.P-471

Electrochemistry

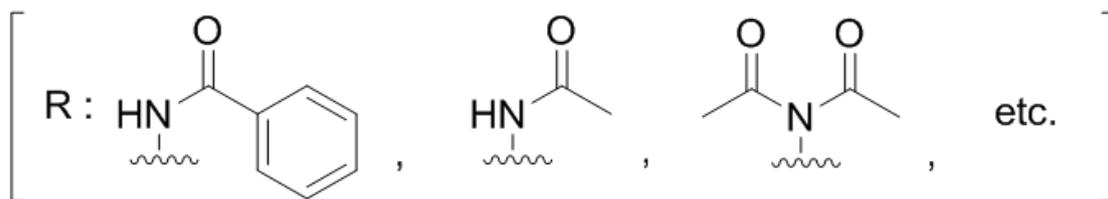
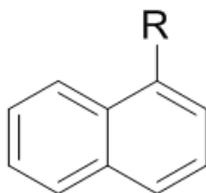
Grand Ballroom, FRI 11:00~12:30

Preparation and Electrochemical Investigation of Naphthalene Derivatives : Apply to Redox Flow Battery

Heung seop Lee, Chujin Ahn*

Department of Chemistry, Changwon National University, Korea

Naphthalene derivatives are interesting to organic anolyte in redox flow batteries (RFB), which have the wide potential windows. In our lab, the functionalized naphthalene derivatives were prepared and investigated their voltage depending on the different functional group with CV.



Poster Presentation : **ELEC.P-472**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Transition metal doped Sb@SnO₂ nanoparticles for photochemical and electrochemical oxidation of cysteine

Yeji Kang, Byung-Kwon Kim*

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Transition metal-doped SnO₂ nanoparticles (TM-SnO₂) were synthesized by applying a thermos-synthesis method, which first involved doping SnO₂ with Sb and then with transition metals (TM = Cr, Mn, Fe, or Co) of various concentrations to enhance a catalytic effect of SnO₂. The doped particles were then analyzed by using various surface analysis techniques such as transmission electron microscopy (TEM), X-ray diffraction (XRD), scanning transmission X-ray microscopy (STXM), and high-resolution photoemission spectroscopy (HRPES). We evaluated the catalytic effects of these doped particles on the oxidation of L-cysteine (Cys) in aqueous solution by taking electrochemical measurements and on the photocatalytic oxidation of Cys by using HRPES under UV illumination. Through the spectral analysis, we found that the Cr- and Mn-doped SnO₂ nanoparticles exhibit enhanced catalytic activities, which according to the various surface analyses were due to the effects of the sizes of the particles and electronegativity differences between the dopant metal and SnO₂.

Poster Presentation : **ELEC.P-473**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Strong Metal-Support Interactions Enhance the Activity of Pd Supported MO_x Electrocatalysts

Wenjuan Shi, Hyun-Uk Park, Ah-Hyeon Park, Jong-Un Jung, Young-Uk Kwon*

Department of Chemistry, Sungkyunkwan University, Korea

The present work reports a general approach to improve the electrocatalytic property of noble metal through regulating its electron status by introducing the strong metal- support interaction (SMSI). As a case study, carbon and metal oxide (Ga₂O₃, Al₂O₃, WO₃) supported Pd nanoparticles were prepared by a sonochemical reaction in the presence of ethylene glycol. For the purpose of comparison, PdM alloys (M: Ga, Al, W) are also synthesized by a revising method. High resolution transmission electron microscopy (HRTEM) and X-ray microchemical analysis were used to characterize the composition, size and distribution of Pd nanoparticles. The electrochemical properties of the catalysts toward oxygen reduction reaction (ORR) and methanol oxidation reaction (MOR) were evaluated using cyclic voltammetry (CV) and chronoamperometry (CA) in 0.1 M KOH electrolyte. The higher catalytic activity for ORR and MOR was increased in the order Pd/MO_x/C > PdM/C > Pd/C. The catalytic activity of Pd/MO_x/C has been significantly promoted by stabilizing Pd species at the interface of the Pd-metal oxide support with the help of SMSI effect, suggesting an intrinsic advantage of Pd in driving ORR and MOR.

Poster Presentation : **ELEC.P-474**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Shape-Controlled Palladium Hydride Nanocrystals as Electrocatalysts for Formic Acid Oxidation

Mrinal kanti Kabiraz, Sang-II Choi*

Department of Chemistry, Kyungpook National University, Korea

The direct formic acid fuel cells (DFAFCs) are promising power source for portable devices, where Pd-based nanocatalysts are most active catalysts toward formic acid oxidation (FAO). Pd- nanocatalysts are more tolerant for CO poisoning, facilitating these catalysts durable over a longer period of reaction for FAO. We have synthesized about ~5 nm PdH cubic and octahedral nanoparticle. Compressive surface strain leading to a down-shift of d-band center observed in CO stripping and XAS measurements for the PdH cubic and octahedral nanocatalysts. PdH cube and octahedra nanocatalysts showed improved activity toward FAO compared with Pd cube, Pd octahedra and commercial Pd black catalyst. The Electrochemical impedance spectroscopy (EIS) measurements during FAO also showed significant improvement of conductivity for PdH cube and octahedra nanocatalysts. PdH cubic and octahedral nanocatalysts were more durable toward FAO operating at 0.4 VRHE than Pd cubic, octahedral, and Pd black nanoparticle.

Poster Presentation : **ELEC.P-475**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Ru branched RuPtCu nanocages as Electrocatalysts for Methanol Oxidation reaction

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The direct methanol fuel cell, one of the most promising energy sources for portable devices and transportation applications, has attracted great attention in recent years. However, the high cost and insufficiency of Pt and the CO poisoning phenomenon during the electrocatalysts considerably inhibited the commercialize usage. Therefore, the synthetic methodology of geometrically and electronically optimized nanocatalyst has been studied. Herein, we introduce the synthesis of hierarchical Ru branched RuPtCu nanocages through the co-reduction of Ru, Pt, and Cu precursors, following the injection of additional Ru precursors. The electrochemical tests show that the catalytic activity and stability of hierarchical Ru branched RuPtCu nanocages for methanol oxidation is much higher than those of RuPtCu/C, PtCu/C, the commercial PtRu/C, and Pt/C catalysts.

Poster Presentation : **ELEC.P-476**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Ultrasonic-assisted Preparation of a Pinhole-free BiVO₄ Photoanode for Improving the Efficiency of Photoelectrochemical Water Oxidation

Joonyong Park, Ki Min Nam*

Department of Chemistry, Mokpo National University, Korea

A pinhole-free BiVO₄ electrode was successfully synthesized using an ultrasonic-assisted synthetic method on a conductive substrate. The pinhole-free BiVO₄ electrode showed highly improved photoelectrochemical activity for both sulfite oxidation and water oxidation. The blocking recombination processes were examined to clarify the enhanced photoelectrochemical performances.

Poster Presentation : **ELEC.P-477**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

The sonochemical preparation of Bi₂O₃/Bi₂S₃ for efficient photoelectrochemical water splitting

Jihyeon Kim, Ki Min Nam*

Department of Chemistry, Mokpo National University, Korea

Photoelectrochemical (PEC) water splitting using semiconductor material has attracted a lot of attention because it is environmental technology which produces renewable hydrogen from water using solar energy. Above all things, Bi₂S₃ has been considered as one of the most promising electrode materials for PEC method due to its narrow band gap (~1.3 eV) and large absorption coefficient. In this paper, Bi₂O₃/Bi₂S₃ was synthesized via simple one-spot sonochemical method. In Bi₂O₃/Bi₂S₃ composite, photogenerated electrons in conduction band of Bi₂S₃ transferred to conduction band of Bi₂O₃, which allow electro-hole pairs to be favorably separated. For this reason, Bi₂O₃/Bi₂S₃ composite show improved photoelectrochemical activity under the visible light irradiation.

Poster Presentation : **ELEC.P-478**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

A Generalizable Top-Down Nanostructuring Method of Bulk Oxides : Sequential Oxygen-Nitrogen Exchange Reaction

Hee-eun Kim, Jin Ho Bang*

Department of Bionano Technology, Hanyang University, Korea

Sequential oxygen-nitrogen exchange (SONE) reaction is developed as a top-down approach to prepare nanostructured oxides from bulk solids. This novel synthesis method that induces grain fracture instead of grain growth at high-temperature is a simple, two-step thermal treatment that is sequentially performed in gaseous NH₃ and in air. The SONE reaction can be applicable to most transition metal oxides and when utilized in a lithium-ion battery, the produced nanostructured materials are superior to their bulk counterparts and even comparable to those produced by conventional bottom-up approaches. Given its simplicity and scalability, this synthesis method could open a new avenue to the development of high performance nanostructured electrode materials that can meet the industrial demand of cost-effectiveness for mass production.

Poster Presentation : **ELEC.P-479**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

FeOF Nanoparticles Wrapped in Graphitic Carbon Layers Derived from Fe-MIL-88B as a Cathode Material for Sodium-Ion Batteries

Achmad Yanuar Maulana, SeonTae Kim, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Lithium-ion batteries (LIBs) have been dominantly utilized as main energy storage systems for electric devices in recent decades. However, the limited resources of lithium and its availability in specific regions have increased its price, making LIBs difficult to be utilized in large-scale applications. Recently, sodium-ion batteries (SIBs) have been considered as a promising alternative due to the abundance, low-cost, and similar electrochemical properties of sodium with lithium. Iron oxyfluoride (FeOF) has been gaining attentions as one of most suitable cathode materials for SIBs due to high theoretical capacity (about 855 mA h g⁻¹), low cost, and low toxicity. However, FeOF has often suffered from poor rate capability and cycling stability because of its low electrical conductivity and ion-diffusion kinetics. In this work, a novel synthetic route to prepare the FeOF nanoparticles wrapped with graphitic carbon layers (FeOF/GCL) was developed by using Fe-containing MOFs (Fe-MIL-88B). During the synthetic process, *in-situ* formed Fe(0) nanoparticles catalyzed the formation of graphitic carbon, and then it was transformed into FeOF through a simple hydrothermal reaction. The FeOF/GCL exhibited the excellent cycling stabilities, discharging the capacities of 467 mA h g⁻¹ at the first cycle and 361 mA h g⁻¹ even at the 100th cycle with a current density of 100 mA g⁻¹ at 1.2-4.0 V. These values are significantly larger than those of bulk FeOF (about 189 and 21 mA h g⁻¹ at the first and 100th cycles, respectively).

Poster Presentation : **ELEC.P-480**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Exploring the Capacitive Behavior of Carbon Electrode Functionalized by Aggregated Cyclic-Edge Ethers

Junghyun Lee, Jin Ho Bang*

Department of Bionano Technology, Hanyang University, Korea

While oxygen-containing functional groups on sp²-carbon structure can enhance capacitance by redox faradaic reactions, they often hinder the access of electrolyte ions, decrease electrical conductivity, and promote energy loss as a form of leakage current. Here, we explored the capacitive behavior of cyclic-edge ether groups introduced onto microporous sp²-carbon monoliths. Unlike oxygen-containing functional groups, the introduction of the cyclic-edge ether group barely distorts sp² carbon network while significantly promoting the accessibility of electrolyte ions. This leads to a superior capacitive behavior, but suppresses self-discharge occurred via parasitic surface redox reactions. In-depth electrochemical impedance spectroscopy provide insight into this novel functionality and implications in the development of nanoporous carbons for supercapacitor applications.

Poster Presentation : **ELEC.P-481**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical and spectroscopic investigations of calcium alloying/ de-alloying with tin for calcium ion battery

Amol Bhairuba Ikhe, Myoungho Pyo*

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Recently, rechargeable calcium ion batteries (CIB) have gained increasing attention as a promising battery systems alternative to lithium-based batteries for grid-scale energy storage. Ca, as an anode material which inherently possesses a number of merits over the alkali metals such as lithium/potassium is safe to use without dendritic growth (like magnesium), high crustal abundant, low cost, and high gravimetric capacity (1340 mAhg⁻¹). In addition, the Ca has a higher reduction potential (-2.87 vs. NHE), which is close to that of alkali metals such as Li and K. The high redox potential and dendrite free nature of Ca are amenable for assembling high voltage and high energy density batteries with suitable cathode materials. However, the passivating behaviors of the Ca in carbonate type electrolytes are similar to that of magnesium, rendering it unsuitable as an anode in CIBs. Alloying of Ca with suitable metals are a promising alternative and previous reports employing this strategy fail to focus on the mechanism of Ca storage at the anode. Herein, we demonstrate the Ca electrochemical alloying/de-alloying with Sn anode for CIB using electrochemical and spectroscopic techniques. In our investigation, we found that the first step of Ca alloying can occur at ca. -1.4 V (vs. NHE). Furthermore, the alloying/de-alloying was confirmed by the XPS, FE-SEM, and EDX mapping. Detailed electrochemical and spectroscopic investigations of the Ca alloying/de-alloying mechanism are underway.

Poster Presentation : **ELEC.P-482**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Calcium Storage in Natural Graphite as an Anode for Calcium Ion Battery

Prabakar Richard, Myoungho Pyo*

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The development in calcium ion battery technology (CIB) has been primarily limited by the difficulties in the lack of a reliable cathode/anode material which is capable of reversible intercalation and de-intercalation of Ca^{2+} ion. The insertion of divalent cation in graphite (Gt) in particular has been difficult due to the high polarization, larger size and energy density of the cations (e.g., Ca^{2+} , Mg^{2+}). Natural Gt which has been well known anode material for Li ion battery has seldom been studied as a suitable anode in divalent ions. Here we report for the first time successful electrochemical co-intercalation of solvated- Ca^{2+} ions in Gt in an ether based electrolyte. The Gt is able to exhibit exceptionally high stability for solvated- Ca^{2+} co-intercalation/de-intercalation at very high rates with a reversible capacity reaching $\sim 60 \text{ mAh g}^{-1}$. We observed the solvated-Ca ion storage mechanism in Gt using in operando X-ray diffraction studies. The formation of various stages was observed with the solvated-Ca ion and was quantified, wherein the highest staging observed was to be stage-2. The configuration of various stages in Gt is proposed by DFT calculation based on the experimental results and calculations explaining the difficulty in the formation of stage-1 type Gt intercalation compound (GIC) and observable capacity are described. The rapid intercalation of solvated-Ca ion in Gt is demonstrated by optical observations, using highly oriented pyrolytic graphite (HOPG), in which the electrochemical intercalation of solvated Ca ions were observed by a corresponding volume increase.

Poster Presentation : **ELEC.P-483**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

A Compromise between Grain Size and Surface Area: Implications for the Lithium Ion Battery Performance of TiNb₂O₇

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Titanium niobium oxide (TiNb₂O₇) has received a great deal of attention in lithium-ion battery (LIBs) because of its high theoretical capacity, environmentally benign nature, and good cycling stability. However, TiNb₂O₇ suffers from limited rate capability due to low Li⁺ ion diffusivity and poor electronic conductivity. In this study, we designed a new synthesis route to prepare monodisperse, mesoporous TiNb₂O₇ microspheres that can mitigate these limitations. Delicate control over annealing temperature offers a way to manipulate the grain size and specific surface area of TiNb₂O₇ microspheres, and our investigation revealed there was a compromise between these structural parameters the LIB performance of TiNb₂O₇ microspheres. This highlights the importance of gaining a comprehensive understanding of the critical factors governing the electrochemical behaviour of TiNb₂O₇ to establish a design principle for advanced electrode materials.

Poster Presentation : **ELEC.P-484**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Novel salt based acetonitrile, propylene carbonate electrolyte systems for high voltage EDLC

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In this study, the new salt 1,1-dimethylpyrrolidinium tetrafluoroborate (DMPBF₄) and well-known electrolytes tetraethyl ammonium tetra fluoroborate (TEABF₄), spiro-1,1'-bipyrrolidinium tetrafluoroborate (SBPBF₄) in acetonitrile (ACN) and propylene carbonate (PC) was systematically evaluated. These electrolytes were firstly investigated by calculation (Gaussian 09) method to achieve the ionic size, solvation energy, interaction energy, reduction, and oxidation stabilities and predict the capacitance. DMP⁺ exhibited the highest solvation energy, interaction energy, smallest ions size drive to lower ionic conductivity so that its capacitance is higher than those of TEA⁺ and SBP⁺. Electrochemical characteristics of those electrolytes such as ionic conductivity, viscosity, cyclic voltammetry (CV), rate capability, and aging test of activated carbon electrode based coin cells was gained. It indicated that influences of the electrolyte components on increasing the capacitance for cells using SBPBF₄ and DMPBF₄ than TEABF₄. The use of ACN as the electrolyte solvent in the cell led to higher capacitance, rate capability than those using alkyl carbonate solvents, such as propylene carbonate. However, through the cycling result, PC showed a little improvement than ACN at 3.0V.

Poster Presentation : **ELEC.P-485**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

N, S-Codoped Mesoporous Carbon Derived from S-Modified Zn-MOF-74 with Enhanced Electrochemical Properties

Dongjun Kim, Geonho Kim, SeoYeah Oh, Wonsik Lee, Jihyeon Park, Jiwon Kim*

School of Integrated Technology, Yonsei University, Korea

As demand in energy storage increases, it is inevitable to develop more efficient energy conversion/storage systems. Accordingly, low-cost and highly active catalysts for oxygen reduction reaction (ORR) and batteries are of a great interest. Porous carbon nanomaterials are attracting attention as promising substitutes for Pt-based ORR electrocatalysts with outstanding stability, high activity, and high electric conductivity. Furthermore, heteroatom doping is an efficient strategy for improving ORR catalytic activity of porous carbon nanomaterials. However, there are still remains a daunting challenge reduce the cost and complexity of synthetic process for heteroatom doped porous carbon materials. Herein, we describe a reliable and controllable synthesis method for low-cost and convenient preparation of nitrogen, sulfur-codoped porous carbon (NSPC). We synthesized a new metal-organic framework (MOF), S-modified Zn-MOF-74, which is highly porous and contains sulfur atoms dispersed homogeneously within the structure. NSPC synthesized by doping the nitrogen and sulfur precursor, thiourea, to S-modified Zn-MOF-74 showed comparable or even better catalytic performance for ORR compared with commercial Pt/C catalysts.

Poster Presentation : **ELEC.P-486**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Altering the catalytic activity by tuning the electronic property of a catalyst via applied external potential

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Catalytic activity depends on electronic nature and steric factors. The catalytic activity is often changed by altering its electronic property. An electron-withdrawing or donating functional group is employed for this purpose. Louis P. Hammett reported the relationship between the reactivity and functional group in 1937, which is then referred as a Hammett principle. Some of the classic examples are hydrolysis of benzoic acid and benzoic ester, which shows how the reactivity was affected by substituents on meta or para position. The substituents affect the reaction by stabilizing or destabilizing the transition states. In other words, substituents alter the electronic property of a reaction center and thus affect the reactivity. The Hammett principle is widely used in several reactions to understand the reaction mechanism. To study the Hammett relationship, functionalization of the reaction center or catalyst is a key part. However, functionalization of the catalysts are often problematic and requires tedious synthetic routes. So developing a new technique to tune the electronic nature of a reaction center would be a fruitful method in catalysis. For this purpose, we introduce a new phenomenon called electroinductive effect. In electroinductive effect, the electronic nature of a catalyst or a reaction center can be altered by an external applied potential within a window that does not involve oxidation or reduction. In theory, positive or negative applied potential would resemble both electron-withdrawing and electron-donating group respectively. To demonstrate the electroinductive effect, we immobilize catalysts on an electrode and illustrate a new way to study Hammett principle. References: Hammett, L. P. J. Am. Chem. Soc. 1937, 59, 96–103.

Poster Presentation : **ELEC.P-487**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Microwave-assisted N, S-Codoped Porous Carbon Derived from Metal-Organic Framework (MOF) as Lithium-Sulfur Battery Cathodes

SeoYeah Oh, Jihyeon Park, Dongjun Kim, Geonho Kim, Jiwon Kim*

School of Integrated Technology, Yonsei University, Korea

Lithium-sulfur (Li-S) batteries have attracted much attention since the demands of rechargeable energy storage devices with high energy density is soaring. Porous carbon is one of the fascinating candidates for Li-S battery cathodes since highly porous structure facilitates penetration of S atoms for activation and absorb intermediate lithium polysulfide.[1] Porous carbon can easily be synthesized by carbonization of metal-organic framework (MOF) with controllable porosity. However, insulating properties of elemental sulfur and intermediate Li_2S , Li_2S_2 causes low utilization of the active material and low retention in the cell cycle. In order to improve the performance, modifying structure and composition (e.g. via doping) of MOF has been actively studied. Heteroatom doping can enhance the conductivity and prevent dissolution of the polysulfide into the electrolyte due to the electronegativity of the doped atoms. Herein, we synthesized MOF-5 derived N, S-codoped porous carbon via microwave-assisted solvothermal method. The microwave-assisted solvothermal process can drastically reduce the time ($^{-1}$) and excellent cell cycle retention of 60% at 0.1 C after 150 cycles. Therefore, we can greatly improve the performance of Li-S batteries (initial capacity and cell cycle retention) by optimizing structure and composition of porous carbon which can contribute to commercialization of Li-S batteries.

Poster Presentation : **ELEC.P-488**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical and spectroelectrochemical properties of terthiophene acrylic acids derivatives

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Three new terthiophene acrylic acids derivatives, 3-(4-([2,2':5',2''-terthiophen]-3'-yl)phenyl)acrylic acid (TTPAA), 3-(5'-(thiophen-2-yl)-[2,2':3',2''-terthiophen]-5''-yl)acrylic acid (TTTAA) and 3-(5-([2,2':5',2''-terthiophen]-3'-yl)furan-2-yl)acrylic acid (TTFAA) were synthesized and confirmed by FT-IR, ¹H and ¹³C NMR, mass spectroscopy. These monomers were synthesized by hydroboration, suzuki coupling reaction, and knoevenagel condensation reaction. UV-visible absorption and PL emission bands of each monomers were observed TTPAA (UV-Vis: 310 nm, PL: 529 nm), TTPAA (UV-Vis: 337 nm, PL: 535 nm), and TTFAA (UV-Vis: 337 nm, PL: 508 nm), respectively. These molecules frontier orbitals showed that acrylic acids functional groups played a role as electron acceptor in terthiophene derivatives. Finally, electrochemically generated conducting polymers were studied by cyclic voltammetry, in-situ UV-Vis spectroscopy, and AFM techniques. Spectroelectrochemical experiments were performed to observe the absorption bands change of new polymers and analyzed by DCVA techniques.

Poster Presentation : **ELEC.P-489**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Development of chromium (VI) sensor using gold-conducting polymer composite electrode

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Sphere Au-poly2,3-diaminonaphthalene(S-Au-pDAN) based composite sensor has been developed for the electrochemical detection of amount of chromium(VI) (Cr(VI)). The modified surface was prepared using a potential step method, where the nanostructured interface showed well-defined voltammetric peak for the reduction of Cr(VI) at ~0.4 V. Proposed sensor was characterized employing electrochemical and surface analysis methods. Experimental variables affecting the analytical performance were optimized. Interference effects of other metal ions having similar redox potentials were also investigated. The dynamic range of square wave voltammetry (SWV) for the target ions were between 10.0 ppb and 10.0 ppm with the detection limits of 1.45 ± 0.15 ppb for the SWV (n = 3). The reliability of the method for point-of-analysis was evaluated by analyzing a standard reference material and various water samples

Poster Presentation : **ELEC.P-490**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Photo-assisted microbial fuel cells using Cu₂O as a cathode assistor.

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Microbial fuel cell (MFC) is a device that can produce electric energy from organic substances. The microbial biofilm on the anode surface converts organic substances into carbon dioxides, protons, and electrons. the most effective way for the anode enhancement is increasing anode surface because it is mainly affected by the amount of the electroactive bacteria on the anode surface. Meanwhile, the electrons from the anode are utilized for the reduction reaction on the cathode surface which is usually oxygen reduction reaction. Although platinum is known as the best material for this purpose, its high price and limited reserve have driven extensive research on alternatives to platinum. In this study, we report a photo-assisted MFC (PAMFC) in an attempt of enhancing power density in which p-type Cu₂O was used as a cathode assistor. Upon illumination of visible light, we obtained power density of 1.4 W m⁻² power density, that is 40% higher without light.

Poster Presentation : **ELEC.P-491**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Novel Methods for Ultra-high Energy Density of Flexible Wire-Shaped Hybrid Supercapacitors

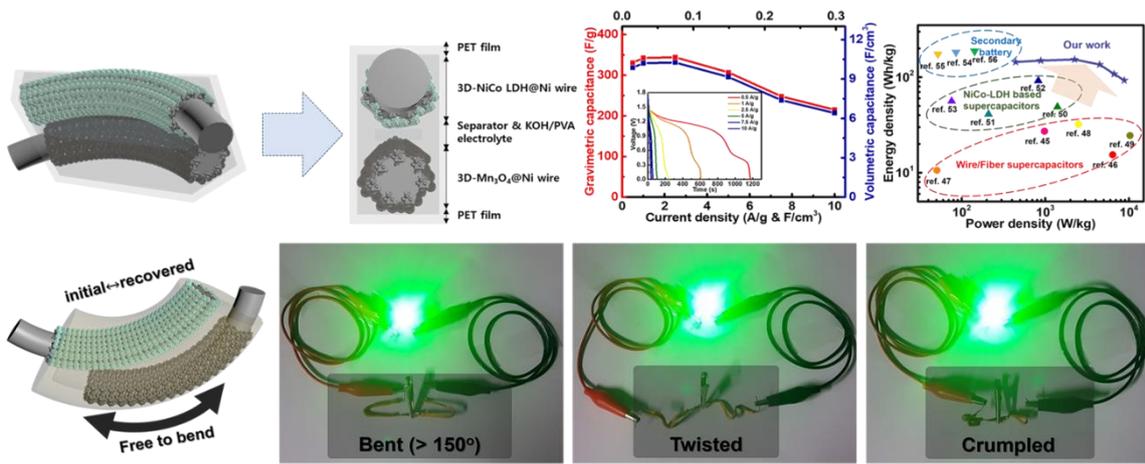
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Wire-shaped hybrid supercapacitors are candidates for flexible wearable applications due to their features of durability under the various deformation conditions, ease of manufacturing, high power delivery ability, fast charge/discharge rates, long cycle life, and low environmental impact. This presentation suggests the novel methods for construction of hybrid supercapacitors with enhanced energy density. A wire-shaped hybrid supercapacitor based on three-dimensional (3D) nickel cobalt layered double hydroxide (NiCo LDH) onto the three-dimensional nickel wire (3D-Ni) with short electron path distances, large electrochemical active sites, and improved structural stability was fabricated as a binder/conductive additive-free electrode for a high-performance supercapacitor. All-solid-state asymmetric supercapacitor achieves a high cell voltage of 1.8V and an exceptional energy density of 153.3 Wh/kg at a power density of 8810 W/kg. Further, the feasibility of the as-fabricated hybrid device was tested in real time conditions by driving LED lights, LCD smart devices, a thermometer, and a wearable watch. The results verified that such wire band-like hybrid supercapacitors are promising for smart wearable and implantable devices having energy delivering capacity and flexibility and might be attractive substitutes for batteries.



Poster Presentation : **ELEC.P-492**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Nanoporous V₂O₅/NiO composite films for electrochromic applications

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Nanoporous V₂O₅/NiO composite films were prepared on flexible conductive substrate by simple wet coating method. The morphology, structure, electrochemical and electrochromic properties of the films were determined by FE-SEM, XRD, cyclic voltammetry and spectroelectrochemistry. Compared with pure NiO and V₂O₅ film, the V₂O₅/NiO composite film showed improvement in cycling stability. V₂O₅/NiO and WO₃ electrode were combined to fabricate a complementary electrochromic device, which showed high contrast ratio, short switching time and excellent durability in Li⁺ gel electrolyte.

Poster Presentation : **ELEC.P-493**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Fabrication of an Amperometric Microsensor for Measurements of Hydrogen Sulfide and Oxygen

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Oxygen (O₂) is the one of the most essential molecules for living organisms. Its supply to a brain through blood flow is regulated carefully by vasodilation and vasoconstriction. Hydrogen sulfide (H₂S) is known to be an important gasotransmitter molecule in the brain, mediating many biological processes including vasodilation. The close interacting dynamics of O₂ and H₂S is an interesting subject to better understand the biological roles of these molecules. In this presentation, we demonstrate the development of an amperometric H₂S/O₂ dual microsensor, which makes it possible to monitor real-time *in vivo* changes in the levels of H₂S and O₂ simultaneously. First, we fabricate a dual electrode having two Pt microdisks of which diameters are 50 μm and 25 μm, respectively. Both Pt micro-disks are electrochemically etched to form recessed micropores, and each micropore is filled with different porous metallic layers through electrodeposition. Then, the electrode surface for H₂S sensing is modified with electropolymerized polymer, while the electrode surface for O₂ sensing is silanized with a gas permeable membrane. The analytical performances of the developed dual sensor are investigated in terms of the sensitivity and selectivity. This highly sensitive and selective dual sensor is enough to be applied in biological environments. 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-2017R1A2A2A14001137).

Poster Presentation : **ELEC.P-494**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Cobalt nanoparticle/sulfur-doped graphene as efficient bifunctional oxygen electrocatalysis in alkaline solution

Jinheui Lee, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Manufacture of highly active electrocatalysts for the oxygen reduction (ORR) and the oxygen evolution reaction (OER) is very important for practical application of fuel cells, metal-air batteries, and electrolyzers. Currently, Pt-based catalysts are regarded as the best ORR catalysts, but not for OER, whereas IrO₂ and RuO₂ are the most efficient catalysts for OER, but poor for ORR. However, the high cost of noble-metal electrocatalysts due to their limited natural reserves has greatly hindered the large-scale commercialization of energy conversion devices. Herein, we report a simple way to prepare a cobalt nanoparticle/sulfur-doped graphene nanocomposite (Co-SGN) as a bifunctional electrocatalyst for the ORR and OER. Benefiting abundant catalytic active sites and unique structural features that influence the exposure of active sites and favor electron transfer, the obtained electrocatalyst exhibits that the ORR and OER on the Co-SGN catalysts proceeded predominantly through the desired 4-electron pathway. The compositional and structural properties were characterized by transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The electrocatalytic activity of the Co-SGN for both ORR and OER was investigated by rotating disk electrode and cyclic voltammetry. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Poster Presentation : **ELEC.P-495**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Semi-quantitative determination of ion transfers at an interface between water and quaternary ammonium polybromide droplets through stochastic electrochemical analysis

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we present stochastic electrochemical analyses for the semi-quantitative determination of ion transfers (ITs) at an interface between water and electrochemically generated quaternary ammonium polybromide (QBr_{2n+1}) droplets (water | QBr_{2n+1}) in QBr aqueous solutions containing different acids (HAs). The concentration of Br⁻ in QBr_{2n+1}, $C_{\text{Br}^-}(\text{QBr}_{2n+1})$ is linearly proportional to $C_{\text{A}^-}(\text{aq})$ with the proportionality constant, which was estimated from the difference between the two partition coefficients of H⁺ and A⁻ from water toward QBr_{2n+1}, $K_{\text{H}^+} - K_{\text{A}^-}$, and the ratio of the mean activity coefficient of the aqueous over that of the QBr_{2n+1} phase, $\gamma_{\pm, \text{aq}} / \gamma_{\pm, \text{QBr}_{2n+1}}$. $C_{\text{Br}^-}(\text{QBr}_{2n+1})$ also shows the linear function of $C_{\text{Q}^+}(\text{aq})$ with $(\gamma_{\pm, \text{aq}} / \gamma_{\pm, \text{QBr}_{2n+1}}) K_{\text{Q}^+}$ as its proportionality constant. The stochastic chronoamperometric analyses of QBr_{2n+1} droplets during their particle-impacts on Pt UME in acidic solutions with MEPBr or EPyBr as model QBrS can provide indirect information about $C_{\text{Br}^-}(\text{QBr}_{2n+1})$, and we estimated the relative order. Also, we found that Br⁻-IT at water|QBr_{2n+1} is effectively limited by A⁻-IT in the acidic solutions, and Cl⁻ is most significantly transferred to QBr_{2n+1}, leading to the complete inhibition of Br⁻-IT into QBr_{2n+1}.

Poster Presentation : **ELEC.P-496**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Revealing indirect electro-reduction of quaternary ammonium polybromide droplets in acidic aqueous solutions

Jiseon Hwang, Jinho Chang*

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In previous work, we electrochemically analyzed stochastic current spikes from Br^- -electrolysis in QBr_{2n+1} droplets by their particle impact on Pt UME. For electro-reduction of QBr_{2n+1} droplets through chronoamperometry, we found no evidence of stochastic current spikes, which are supposed to be evidence for direct electro-reduction (DR) of QBr_{2n+1} droplets to Br^- and Q^+ through their particle impact on Pt UME. Instead, we suggest an indirect electro-reduction (IDR) mechanism for QBr_3 droplets. QBr_3 equilibrated with Q^+ and Br_3^- and the liberated Br_3^- from QBr_3 droplets are electrochemically reduced to Br^- until all the QBr_3 droplets in the vicinity of the Pt UME are depleted. We further found that QBr_{2n+1} species ($n = 2$ and 3) are not electro-reduced through IDR but are precipitated on Pt UME. The frequency of the current spikes in the $CA_{\text{forward-50 cycles}}$ significantly declined as the potential-cycles increased. The chronoamperometric analyses indicated that the Pt surface is partially blocked by the reduction-inactive QBr_{2n+1} species, which was confirmed to be mostly QBr_5 and QBr_7 by Raman spectroscopy.

Poster Presentation : **ELEC.P-497**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Synthesis of Co₂Si nanowires on silicon substrate for on-chip electrochemical capacitor application

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Electrochemical capacitors have received great attention because of their high power capability, excellent cycle stability and high charge/discharge rate. Among various materials, metal silicides have potential for use as electrode materials for electrochemical capacitors due to their high electrical conductivity, high earth abundance, and potential ease of integration into conventional silicon-based electronics. Herein, Co₂Si nanowires with small diameters of ~20-70 nm have been synthesized on silicon substrate by using simple chemical vapor transport method and their electrochemical performance for the electrochemical capacitor has been investigated. The as-synthesized Co₂Si nanowires show high areal capacitance, high energy density, and good cyclability in an ionic liquid electrolyte. We suggest that Co₂Si nanowires have great potential as electrode materials for electrochemical capacitors.

Poster Presentation : **ELEC.P-498**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Binary metal nanoparticles embedded in carbon nanofiber for efficient electrochemical water splitting

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Developing low-cost and efficient electrocatalysts for hydrogen evolution reaction (HER) and oxygen evolution reactions (OER) are one of the major challenges for electrochemical water splitting. Herein, we report achieves a series of metal-based nanoparticles (Co–CeO₂, Ni₂Fe) embedded in carbon nanofibers (CNFs) by using electrospinning technique and heat treatment process, which are found efficient catalysts for electrolytic water splitting. The Co–CeO₂ embedded in CNFs (Co–CeO₂@CNFs) and Ni₂Fe embedded in CNFs (Ni₂Fe@CNF) produce low overpotentials of 92 and 239 mV at a current density of 10 mA cm⁻² as catalysts for HER and OER, respectively. The as-prepared hybrid materials demonstrate outstanding catalytic activities as non-noble metal electrodes rendered by the synergistic effect of bimetal elements and the improved electrical conductivity. With the use of these Co–CeO₂@CNFs and Ni₂Fe@CNF catalyst, an alkaline water electrolyzer in a two-electrode configuration achieved 10 mA cm⁻² only at a cell voltage of 1.55 V with iR compensation in 1 M KOH. Our results suggest that the metal-based nanoparticles (Co–CeO₂, Ni₂Fe) embedded in CNFs could serve as a low-cost, highly active catalyst for electrochemical water splitting.

Poster Presentation : **ELEC.P-499**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

In-depth study of on Single Nanocavity Electrodes

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Recently, there are several papers about unprecedented behavior on nanoelectrodes. There are some attempts to understand nanoelectrochemistry (e.g. collision of nanoparticles on a microelectrode and investigation on electrochemical behavior on nanoelectrodes prepared by lithographic techniques. In this study, nanocavity electrodes with controlled pore diameter and height of surrounded insulation layer were fabricated by photolithography and focused ion beam. To fully understand nanoelectrochemistry on these electrodes, redox behavior was intensively studied according to scan rates, concentrations of redox species, kinds of redox species, kinds of supporting electrolyte and concentrations of supporting electrolytes.

Poster Presentation : **ELEC.P-500**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical Determination of Dopamine with V_2O_5 - WO_3 Composite Nanotube

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Dopamine (DA) is a vital modulator in nature, working especially as hormone and as neurotransmitter in human body. Direct detection of DA is sometimes necessary for clinical purpose and we herein provide amperometric sensing of DA using electrospun V_2O_5 - WO_3 composite nanotube (VW NT). We prepared VW NT with various ratios of V and W precursors via electrospinning followed by calcination. To improve sensitivity we tried further by reducing VW NT with hydrogen or irradiating VW NT with UV light. The change of the morphology and oxidation states of VW NT, before and after hydrogen reduction or UV irradiation, was characterized by field emission scanning electron microscopy (FE-SEM) and X-ray powder diffraction (XRD). To investigate the variation of electrochemical properties for DA measurement depending on treatment of VW NT, we used cyclic voltammetry, rotating disk electrode voltammetry, and amperometry. We also tried to circumvent the interference of other species (i.e., glucose, ascorbic acid, acetamidophenol, and uric acid). The support of this work by NRF-2017R1A2B4002159 is gratefully acknowledged.

Poster Presentation : **ELEC.P-501**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Meso-scale Rh electrocatalysis for hydrogen evolution reaction in acid condition

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Hydrogen is expected to be one of the most important energy sources to solve the environmental and energy critical situation due to its high energy density and little environmental pollution. There is a well-known volcano-type relationship between energetics and current density for hydrogen evolution reaction (HER) catalysts. The Pt-based catalysts located on the top of the volcano considered as the most effective ones. Nevertheless, the major drawback of Pt based catalysts is their high cost. So, it is significantly important to design and synthesize another metal-based efficient catalysts to substitute Pt catalysts. In this study, meso-scale Rh structures have been employed for HER. It is expected to show highly catalytic activity because it has abundant exposed active sites and highly accessible surfaces. And electrochemical performances of meso-scale Rh catalysts such as kinetics, electrochemical surface area, lower electrochemical resistance, and durability is intensively studied comparing at different pH electrolyte conditions.

Poster Presentation : **ELEC.P-502**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Electrochemical modification of diazonium for highly sensitive impedimetric DNA sensor

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Electrochemical DNA sensors offer simple and rapid tools for detection of DNA sequences or damaged genes associated with human diseases. The performance of electrochemical DNA sensors is critically dependent on the process of the DNA immobilization. In this study, 4-nitrobenzenediazonium was chosen as a diazonium compound and electrochemically modified on a gold electrode. Unlike thiol-based self-assembled monolayers, electrochemical reduction of diazonium is a more selective and desirable strategy in a view of resistance to electrochemical perturbation and long-term stability. Then nitro group was converted into amino group through electrochemical reduction processes. After glutaraldehyde treatment, probe DNA sequence for Dengue virus was finally immobilized for detection of target DNA. All processes were electrochemically monitored using cyclic voltammetry and electrochemical impedance spectroscopy of ferri/ferrocyanide.

Poster Presentation : **ELEC.P-503**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Application of electrochemical biosensor using ferrocene-containing redox antibiofouling polymer

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Korea*

A ferrocene-containing multifunctional redox copolymer synthesized by radical polymerization for application of electrochemically active layer on an indium tin oxide (ITO) electrode. The surface adhesive monomer acts as an anchor to the ITO surface, the polyethylene glycol (PEG) group acts as an antibiofouling functional group, the epoxide group selectively conjugates antibodies on the polymeric ITO surface, and the ferrocene group is the redox-active compound for electron mediator. The ferrocene-containing polymer exclusively produced a distinguishing redox wave due to ferrocene, as opposed to the ferrocene-free polymer. To further demonstrate the usefulness of our polymer systems, we configured a sandwich immunoassay; the ferrocene-containing polymer largely improved the sensitivity and dynamic range of the immunoassay as compared to the ferrocene-free polymer.

Poster Presentation : **ELEC.P-504**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Development of electrochemical biosensor for detection of human norovirus based on 2-dimensional material

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The harmfulness of norovirus, which can cause acute foodborne gastroenteritis, has increased worldwide because even at 10² copies/mL or fewer virus particles in the human body can trigger the disease. The primary reason for infection by this virus is closely related with the ingestion of contaminated shellfish, thus, highly sensitive and selective diagnosis tools are needed. Although there are many types of detection methods were considered in this study, the electrochemical biosensor was introduced for its sensitivity and reproducibility. Two-dimensional (2D) materials such as graphene or transitional dichalcogenides have attracted many researchers due to their superior properties on strength, stability, conductivity and biocompatibility. The thin film of MoS₂ and WS₂ are emerging electronic materials which show the high electrochemical properties. In this work, the development of WS₂ nanomaterial morphology has been instituted by using hydrothermal method. Then, a cooperation of gold nanoparticles (AuNPs) on WS₂ has been used for electrochemical detection of norovirus. The performance of the specific peptides has been studied with fluorescent optical assay, and gold-doped WS₂-immobilized synthetic peptides have been studying cyclic voltammetry (CV) and impedance spectroscopy (EIS). These results demonstrated the potential of biosensor based on 2D materials in cooperation with AuNPs for the norovirus detection. The use of 2D materials promises the available in various of biosensing platform for point-of-care testing.

Poster Presentation : **ELEC.P-505**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Preparation of hexagonal sodium tungsten oxide nanoflowers: Their various application for detecting H₂O₂ as enzyme-like mimics and electrocatalysts

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Sodium tungsten oxide nanoflower (WONFs) is prepared through a simple hydrothermal reaction at low temperature. Tungsten oxide has been widely studied due to its electro-chromic and -catalytic properties such as peroxidase-like activity, which decomposes hydrogen peroxide to H₂O molecule and electron. Because the catalytic activities occur on the interfacial, the surface area and morphology of catalyst are closely related to their activity. Among the several structures, nanoflower shape has known that it has larger surface area per unit volume than sphere or rod shape. The main object of this research is to synthesize the products and monitor their electrochemical detection activity. The sample was characterized by XRD, TGA, DSC, SEM, TEM, EDX, FTIR, XPS, BET and electrochemical analysis such as CV and chronoamperometry. Peroxidase-like activity of WONFs were investigated to two ways, first is colorimetric methods, with detection limit of 138 μ M, and second is electrochemical analysis with detection limit of 56 nM. In colorimetric detection, 3,3',5,5'-tetra-methylbenzidine (TMB) was used and in electrochemical detection, modified glassy carbon electrode (GCE) was used. Based on the above results, it was revealed that the products have flower-like shaped Na_{0.17}W_{3.085}O_{0.17}H₂O and peroxidase-like activity. In addition, it can be applicable to H₂O₂ detect biosensor platform due to their electrochemical property and high selectivity.

Poster Presentation : **ELEC.P-506**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

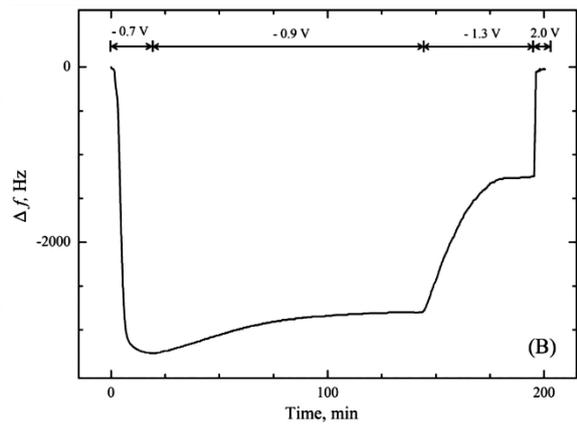
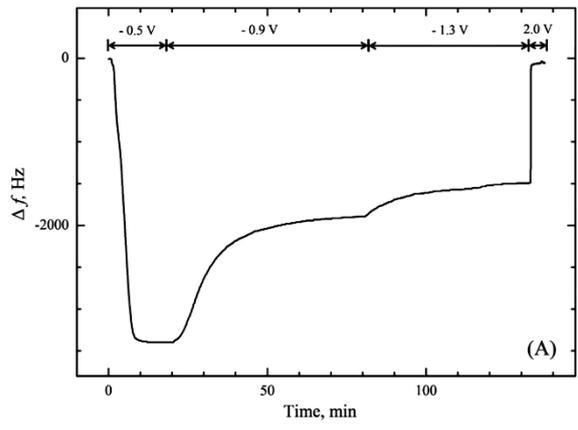
Compositional Analysis of Electrodeposited Cobalt Selenide Thin Films Using Continuous Flow Electrochemical Quartz Crystal Microgravimetry

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In this study, the composition of electrosynthesized cobalt selenide thin films was analyzed by electrochemical quartz crystal microgravimetry (EQCM) in a continuous flow mode. First, cobalt selenide films were electrodeposited on a Pt-EQCM electrode using a 0.1 M Na₂SO₂ electrolyte solution containing Co and Se precursor species at different potentials. A combination of sequential stripping and EQCM frequency monitoring protocol enabled mapping of the free Co, free Se, and CoSe content of the electrodeposited films. It was found that the composition of cobalt selenide film was very sensitive to the electrodeposition potential. The targeted CoSe content was maximum at -0.7 V and the free Co content was minimum at this potential. On the other hand, the free Se content decreased from ~45% at -0.6 V to nearly 0% at -0.9 V. The film composition as established by the continuous flow analysis mode stood in stark contrast with the static (batch) mode where no free Co was observed in the films. Factors in these compositional differences as well as in the EQCM electrode geometry (face-down vs. face-up) are finally discussed.



Poster Presentation : **ELEC.P-507**

Electrochemistry

Grand Ballroom, FRI 11:00~12:30

Oxidation Power Enhancement of Hypochlorite by pH-Control

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Hypochlorite, which is widely used as an oxidizing agent for disinfection, could be increased in oxidizing power by pH-control. The increased oxidizing power was confirmed by the potentiometry, and the cyclic voltammetry was used for confirming the reduction potential change of hypochlorite ion. The reduction-oxidation potential (ORP) was positively shifted at pH 7 or below. In cyclic voltammogram, the reduction potential of hypochlorite was observed around -0.2 V and shifted to +0.3 V after the addition of a citric acid or hydrochloric acid. The enhanced oxidizing power of the mixtures was confirmed by a 5-minutes contact disinfection test of harmful bacteria (*Escherichia coli* and *Staphylococcus aureus*), in which the concentrations of hypochlorite were 40 ppm.

Poster Presentation : **EDU.P-486**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Understanding the Experience of Overseas Educational Volunteer Activity from Analyzing the Students' Report

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Korean pre-service teachers went to Nicaragua and taught elementary and secondary students last winter. The purpose of this study is to understand the meaning of this overseas educational voluntary activity. The author led the pre-service teachers to prepare the voluntary activity, managed the whole activity in Nicaragua for four weeks, and wrote the final report of the activity. The pre-service students (N=17) submitted their own reports which described what they have experienced in the voluntary activity. For the analysis of students' report, this study used the Net-Miner. Net-Miner is one of the software used in the analysis of big data. Students' reports consist of 13416 words, 2028 sentences, and 367 paragraphs. Net-Miner produces the 'word cloud' that shows the most frequently used words. The word cloud contained the words such as 'lesson', 'thinking', 'voluntary', 'student', 'preparation', 'time', 'education' etc. In the 'topic modeling' some main topics can be derived. The derived topics can be described as 'thinking on the meaning of voluntary activity in Nicaragua', 'children and students in school time', and 'preparing and giving lesson in Spanish.' I will discuss the possibility and usefulness of big data analysis as a complementary tool in a qualitative research.

Poster Presentation : **EDU.P-487**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

THE UNDERSTANDING OF BACKGROUND OF 2017' REVISED JAPANESE SCIENCE NATIONAL CURRICULUM (2)

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This study has reviewed overall issues of the Japanese science education based on (i) the analysis of the research on the domestic and international surveys for academic achievements and (ii) the on-site research of the elementary, middle and high schools, and has looked into the fundamental principles of the newly revised Japanese science curriculum and the influence and relevance of the issues of the Japanese science education to the revision of the science curriculum. In this study, the analysis of the research on the domestic and international surveys for academic achievements and curriculum, which is concerned with the science subject conducted under the current Japanese curriculum, is categorized into the international and the domestic research results, and which are further categorized into (A) the aspect of scientific learning achievement and the scientific learning contents, (B) the aspect of students' attitude on science, and (C) the aspect of the environments for science education.[1] Y.T. Kong (2011). The Understanding on the Revised Japanese Science Curriculum. *Subjective Education Research*, 15(1), 123-142.Acknowledgments: This work was supported by National Research Foundation of Korea Grant funded by the Korean Government (NRF-2016R1D1A1B02008712).

Poster Presentation : **EDU.P-488**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Analysis of modeling process of science gifted students: Focusing on evaluation of model

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The education using science modeling as a method of scientific communication and science practice has recently attracted attention in science education. In this study, five students of K gifted school saw the video clip about changes after candle burning. Since then, they have been asked to create their own model that can explain this phenomenon. This study focuses on how to evaluate their models through observations of coincidence or non-coincidence in the process of verifying the models established by the students themselves. As a result of the study, there were two types of cases in the evaluation of the model. First, it is a type that firmly keeps the model with firm belief in the model that it establishes regardless of observation fact. The second type had no firm belief in the model it established relatively. So students of this type discarded or modified the model by observing new facts during the verification of the model. The model is not discarded or modified as a single observation case. But there is no absolute science model. The model should always be the subject of evaluation and the discrepancy between the actual experimental results and the model's predictions is important as criteria of the evaluation. While the evaluation of the model should have a balanced view of these two perspectives, the gifted students had only one. Gifted education is aimed at cultivating scientists to create science models in the future. As shown in this study, the gifted students are lacking in scientific competence. In order to become a gifted education capable of cultivating a scientist, we suggested that education on science models including modeling should be directly reflected in gifted education with getting out of the framework of existing accelerated learning.

Poster Presentation : **EDU.P-489**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

A Study on the Change of Thinking of pre-service Teachers through the Experience of Secondary School Applying Responsive Teaching Methods

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The purpose of this study was to identify the effect of responsive teaching methods for pre-service teachers in Chemistry Education Department of H University. We designed three steps for the education: foregrounding the substance of students' ideas, recognizing the disciplinary connections within students' ideas, taking up and pursuing the substance of thinking. In the step of foregrounding the substance of students' ideas, we analyzed the questionnaires conducted by the 20 pre-service teachers to understand the substance of students' ideas about boiling and evaporation. Among them, five pre-service teachers were selected to recognize the disciplinary connections within students' ideas. Through these steps, the pre-service teachers have grasped the substance of their thinking about boiling and evaporation, and have experienced the process of correcting or pursuing the frames of thought by the disciplinary connections within students' ideas. The effects of responsive teaching methods in pre-service teachers' education are as follows: First, by recognizing differences in prerequisites, pre-service teachers were able to obtain the ability to find seeds that could be linked to discipline. This will enable us to recognize the importance of creating a flexible curriculum that can be linked to discipline from students' thinking, away from the role of existing teachers. Second, pre-service teachers became aware of the importance of the value of thinking process change rather than scientific knowledge or result-oriented performance, and of the importance of teaching ability to develop students' abilities. Therefore, it is necessary to emphasize a responsive teaching method as one of the teaching methods that can enhance a student's ability in pre-service teacher education.

Poster Presentation : **EDU.P-490**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Analysis of Textbooks on Electrolysis Experiments of Electrolyte Aqueous Solution and Conclusions on Electrolytic Electrolysis of Gifted Students

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Electrolysis of electrolytic aqueous solution produced H₂ and O₂ at the (-) and (+) poles, which is an experiment that revealed that water is not an element but a compound. In addition, electrolysis of aqueous solutions is presented as a different motivation in different units of various subjects. In this regard, we analyzed eight middle school textbooks, four kinds of chemistry I, and four kinds of chemistry II. The questionnaires were asked to students of gifted students about the relationship between electrolytic phenomena and electrolysis phenomena. In addition, students were asked to analyze the results of electrolysis experiments of aqueous solutions and their interpretations. In Science 2, experiments were carried out in the same manner as electrolysis of electrolytic aqueous solution to explain the principle of current flow in aqueous electrolyte solution. However, only the movement of ions was concerned and the presence of water and the electrolysis process at each electrode were omitted. As a result of analyzing 8 textbooks, only one kind of textbook and teacher's guidebook mention the possibility of electrolysis of aqueous solution. Of the students who responded to the questionnaire, 45% of the students explained the current flow in the electrolytic aqueous solution as a consumptive model that considers ion migration only. Electrolysis experiments of electrolytic aqueous solutions are handled twice in the same unit with different motions. Nevertheless, it can be interpreted that the opportunity to look at the phenomenon as a whole is not provided because of focusing on each learning objective. In order to explain that electrons are involved in chemical bonding in Chemistry I, the textbook presents electrolysis experiments of NaOH (aq) and Na₂SO₄ (aq), and exploration experiments to confirm that the volume ratio of hydrogen and oxygen produced is 2:1. Two kinds of chemistry I guidebooks, three kinds of chemistry II textbooks, and four kinds of teacher guidebooks list the kinds of ions that are less oxidizable and less reducible than water considering only the standard reduction potentials, and present the expected experimental results uniformly.

In addition, it ignores the role of electrolytes in all chemistry II textbooks and teacher guides, and suggests a kind of unified mechanism in which water molecules are directly electrolyzed from both electrodes. As to the different electrolysis results of NaOH (aq), Na₂SO₄ (aq), and KNO₃ (aq), the students interpreted that the product was dissolved in water rather than attempting a bold interpretation that different kinds of products were produced at the electrode Or interpreted as experimental error. This can be interpreted as indirect evidence that students are accepting textbook descriptions truthfully because of a uniform science description.

Poster Presentation : **EDU.P-491**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

A Case Study on Teacher Instruction Expertise through the Teaching and Learning Community

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One of the factors affecting student achievement is the professionalism of the teacher, and developing the professionalism of the teacher is important to improve the quality of education. Teacher professionalism has a decisive influence on the quality of education, and no education reform can succeed without teacher change. The knowledge, skills and expertise that science teachers need to have become more important than before. Teacher variables were found to have a greater effect on student achievement than any other single factor, including class size, parent education, income level, and language background. In the past, the direction of professional development, which emphasized education and training for teachers, has recently been shifted toward professional development through collaboration with colleagues. From this point of view, this study examined the 'Teachers for Exiting Science'(TES), a science learning community in Seoul Gyeonggi province. To do this, we surveyed the status of the meetings, analyzed their online communities, and took classroom classes to assess the professionalism of the participating teachers. Most of the participating teachers who participated in the TES participated in the TES for sharing and experimenting with the data, and they were satisfied with the new book, and the expertise of the expression area and the teaching method was improved through the meeting. In order to analyze the activities of TES's activities, active interaction was taking place in the private online community of TES teachers, and the biggest function was 'sharing friendship' and 'sharing of information' It is understood that they participate for the purpose of emotional exchange and professional development with fellow teachers. As a result of evaluation of instructional expertise through classroom observation and video analysis, the highest level of achievement was shown in 'Interaction and Respect' factor, and the teachers of 'excellent' class were veteran teachers with long experience of learning community activities. They were using a variety of teaching resources, designing meaningful learning programs, and actively engaging in meaningful interaction with students. On the other hand, the teachers who are in 'beginners' class did not have diverse resources due to

their lack of experiences and experiences, and they were in a rigid type of less flexible interaction with students and less positive interaction with students. As a result of the questionnaire survey of the TES on the present curiosity, it was pointed out that the activity direction of the curiosity center, the quality deterioration of the development data level and lack of fellowship between the TES should be improved. In addition, as the merits of TES, it was often accompanied by fellow teachers who share professionalism and meanings. In the future, TES to develop and disseminate teaching and learning materials to achieve the goals of 'exciting science', 'to develop professionalism to achieve precise science goals, and to achieve the goal of science for all' I heard the popularization of science for. In this study, we surveyed the status of the new science learner, a representative science teacher learning community in Korea, and the teaching expertise of participating teachers. TES is a learning community that has been actively engaged for 25 years to achieve three goals and consists of teachers who are constantly striving to improve their professionalism. Most of the teachers, who consistently and enthusiastically participated in the Divine Comedy, were highly evaluated in the assessment of their professionalism in class, and their participation was the cause. The teacher-learning community, in which teachers are voluntarily engaged, has a great influence on the professional development of the teacher. Such meaningful efforts must not only continue to develop but also make a meaningful voice to the scientific education one step further the learning community in Korea.

Poster Presentation : **EDU.P-492**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Development and Application of STEAM Program about Dokdo Island to Middle School Students

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In this study, the STEAM program about Dokdo Island was developed and applied to 151 middle school students from 5 schools in Daegu and Gyeongbuk region. Teaching and learning materials for STEAM Program about Dokdo Island covers scientific facts, safe transportation method, ecological value, structure and properties of gas hydrate buried in Dokdo during four class hours. Before and after instruction, questionnaires about the attitude toward STEAM program. Students' knowledge and perception of Dokdo Island, and questionnaire of science-engineering career choice were also surveyed. As a result, the program positively influenced students' knowledge and awareness of Dokdo Island and confirmed the significant effect on the improvement of attitudes toward science classes and awareness of science and engineering career. Based on these results, educational implications were discussed.

Poster Presentation : **EDU.P-493**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

The Relationship between Mentor Teachers' Mentoring Characteristics and Mentee Teachers' Reflective Practice in Collaborative Mentoring

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The purpose of this study was to examine the relationship between mentor teachers' mentoring characteristics and mentee teachers' reflective practices in addition to determining mentor teachers' methods of mentoring to enhance mentee teachers' reflective practices. Participants of this study were four mentee teachers and four mentor teachers who participated in the collaborative mentoring program, as well as a research team that consisted of a professor as an expert of science education, a doctorate candidate, and a Ph.D student in science education who is also a researcher of this study. The collaborative mentoring program was managed by arranging four mentee teachers with less than two years of teaching experience and four mentor teachers into four pairs. The conceptual elements of the collaborative mentoring program applied in this study - 'Communication Skill', 'Pedagogical Content Knowledge(PCK)', 'Reflective Thinking', and 'Reflective Practice' - were represented in four activities titled 'One-on-one Mentoring', 'Seminar and Workshop', 'Self-evaluation' and 'Discussion'. One-on-one mentoring, the core of the collaborative mentoring program, was performed five times. One-on-one mentoring provides mentee teachers the opportunity to reflect, after they have been given feedback on their actual classes by mentor teachers. This study compiled mentor and mentee teachers' journals, records and transcripts from mentee teachers' five periods of classes, lesson plans, evaluation forms of lessons, one-on-one mentoring records and transcripts, questionnaires conducted before, during, and after the mentoring program, and a questionnaire about the effects of one-on-one mentoring. The mentoring characteristics of mentor teachers' were analysed quantitatively based on interaction methods with mentee teachers in one-on-one mentoring conversations, content of teaching feedback and feedback frequency from mentor teachers. A qualitative analysis was performed focusing on cases that exhibited mentoring characteristics. Mentee teachers' reflective thinking was assessed for self-reflections of their classes and reflections on the support provided by mentor teachers. Mentee teachers' reflective practices were analysed quantitatively through RTOP; a

qualitative analysis was carried out based on mentor and mentee journals and a questionnaire about the effects of one-on-one mentoring. The conclusions of this study are as follows. Firstly, mentor teachers can improve mentee teachers' reflective practices by facilitating conversation that helps mentees perceive problems in their teaching practices. According to the results of the study, mentee teachers' self-reflection influenced their reflections on support provided by mentor teachers' and generally led to reflective practices. Therefore, mentoring that assists the development of mentees' self-reflection should be supplied in order to encourage reflective practices regarding support provided by mentor teachers. Mentee teachers' self-reflection depended on mentor teachers' methods of interaction. When mentor teachers applied unilateral and directive mentoring, self-reflection rarely occurred. However, when mentor teachers encouraged mentee teachers to discover problems on their own, using questions that promote reflective thinking, self-reflection was volunteered more regularly. Secondly, when mentor teachers give feedback, this support helps mentee teachers identify and solve problems by themselves and encourages mentee teachers' reflective practices. The teachers who reflected on problems existing in their own classes practiced reflection well, although not every case of reflective thinking led to reflective practices. Reflective practices rarely materialized when mentee teachers were asked to solve problems without aid from mentor teachers because of the lack of PCK. However, when mentor teachers helped mentee teachers find solutions during mentoring conversations, mentee teachers were able to solve problems by themselves, and as a result, mentees practiced reflection more frequently. Thirdly, mentee teachers' reflective practices can be encouraged when mentor teachers specifically emphasize reflective thinking. Although mentor teachers were unable to elicit voluntary reflection from mentee teachers due to their lack of strategies, when mentor teachers specifically emphasized reflective thinking, mentee teachers' reflections on support from mentor teachers occurred frequently. Lastly, mentee teachers' reflective practices can improve through continuous communication between mentor teachers and mentee teachers. Mentee teachers practiced reflection more often when they expressed the kind of support they desired from mentor teachers and when mentor teachers evaluated their own mentoring methods by constantly checking that mentee teachers were being helped by their mentoring. Mentee teachers' reflective practices did not improve when their requests for support were ignored or when mentee teachers were unable to easily communicate the kind of support they desired to the mentor teachers.

Poster Presentation : **EDU.P-494**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

The Effect of Teacher's Written Feedback on the Quality of Argumentation in Students' Claim and Evidence Writing in Inquiry chemistry Experiment

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The purpose of this study is to investigate the effect of teacher's written feedback on the quality of the argumentation on students' claim-evidence writing. In this study, 31 students from the Science Education Department of the Teachers College participated in the 'inquiry chemistry experiment'. The students in the experimental group and the comparative group performed all the other activities in the same way, except that they provided written feedback. In the experimental group and the comparative group, pre- and post-claim-evidence writing test for the candle experiment and electrolytic experiment (Da eun Kim, 2014) were conducted. And the students of experimental group conducted interviews and awareness questionnaires about the teacher's written feedback after post-claim-evidence writing. The results of the study are as follows. First, the results of the SPSS 25.0 analysis of the pre- and post-claim-evidence writing test score of the experimental group and the comparative group, in comparison within the group, the experimental group showed significant improvement in the claim, evidence score of candle experiment, and the evidence score of electrolytic experiment except the claim score of electrolytic experiment, whereas the comparative group showed significant improvement only in the evidence score of electrolytic experiment(p

Poster Presentation : **EDU.P-495**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Analysis of students' self-assessment and teachers' assessment of students' character competence based on the Collaborative Problem-Solving for Character Competence instruction model

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Aiming for understanding students' character competence enhanced by the Collaborative Problem-Solving for Character Competence(CoProC) instruction model, this research analyzed students' self-assessment and teachers' assessment of students' character competence with the qualitative assessment tool of which nine elements including openness, sympathy, tolerance, consideration, sincerity, self-control, honesty, responsibility, and cooperation were adopted, developed by our previous research. Through experts' discussion and pre-survey, the new qualitative assessment tool was elaborated, resulting in 53 checklists. Teachers were observing pupils' dialogue and behavior with the tools, while students were checking their recognition with the same tools. Both data were compared and analyzed.

Poster Presentation : **EDU.P-496**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Analysis of Inquiry Status of the Lower-level and the Higher-level Middle School Science Textbooks of Kim Jong-Un Era in North Korea

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In 2013, DPRK announced the ‘General 12-Year Obligatory Education Doctrine’ and compiled a new textbook in the Kim Jong-Un system. Kim Jong-Un education aims “nurturing a talent with a sound thinking ability, a deep knowledge of science and technology, and a strong physical strength.” DPRK emphasizes intelligence education not only to acquire simple knowledge but also to improve intellectual ability, thinking ability, and knowledge inquiry method, and pursues to nurture "creative" and "practical" talents through education. And the proportion of natural science subjects such as natural sciences, physics, chemistry, and biology in the secondary curriculum has greatly expanded compared to other subjects. Also, DPRK emphasizes education of the development of independent learning ability and creative ability, and experiment practice for nurture science and technology talents to lead ‘Knowledge Economy Power Nation.’ At the 7th Workers’ Party Convention, DPRK’s Education Policy has been shown to encourage students’ to inquiry activities in teaching-learning process, emphasizing inquiry learning for creative human development and encourages students’ inquiry activities in teaching-learning process. The purpose of this study was to analyse the inquiry status of science textbooks of the Kim Jong-Un era in DPRK using the Romey’s framework to understand the science education in North Korea and provide it as basic data of science education to prepare for unification of Korean Peninsula. Romey’s framework consisted with texts, contents, pictures, diagrams, questions of the science textbooks. The lower-level and the higher-level middle school science textbooks were quantitatively analyzed by Romey’s framework. The fact that textbooks of all grades in DPRK were not available was a limitation of this study.

Poster Presentation : **EDU.P-497**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Comparative analysis of evaluation questions presented in Korean chemistry textbooks and North Korea chemistry textbooks

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The purpose of this study was to analyse evaluation items presented in Korean chemistry textbooks and North Korea chemistry textbooks. We decided the classification of Klopfer to analyse the textbooks. We quantified the distribution of questions according to each category through this study. Results were follows as: First, chemical textbooks of 2015 revised National Science Curriculum in South Korea's have many questions that were related to real life and could foster creativity. Second, there were mostly knowledge transfer-oriented questions in North Korea's chemical textbooks rather than creative questions. It is judged that if a unified textbook is created, it will not be able to be integrated at once due to the wide gap in the inter-Korean curriculum. Therefore, it would be possible to create a unified textbook for each level and integrate the entire curriculum with the textbooks, assuming that they will be gradually integrated into one.

Poster Presentation : **EDU.P-498**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Study on the Changes in North Korean Higher-level Middle School Chemistry Textbooks before and after the Kim Jong-un era

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The purpose of this study was to investigate changes in North Korean chemistry education through analyzing chemical textbooks before and after the Kim Jong-un era. In this study, chemical textbooks used in upper grades of middle school before 2013 and higher-middle school chemistry textbooks of Kim Jong-un in 2013 were analyzed. Analysis frame of chemistry textbooks were as follows: educational objectives, contents, structure, evaluation items, activities, characteristics, and so on. As a result of analysis of chemical textbooks, first, chemistry textbooks was similar to the chemistry textbook before Kim Jong-un era as chapter, unit, sub-unit, but the title of chapter and unit were presented as questions. Second, the characteristics of the textbooks were not education in a way of transmitting knowledge, but it was a kind of education through the learning activities such as 'student activity,' 'discussion,' 'thinking,' 'explanation', 'experiment', and etc. Third, textbooks briefly introduced the characteristics and goal of chemistry subjects and how to learn chemistry well, and explains scientific inquiry methods, and followed a series of inquiry processes along with the proceed of textbooks. The result of this study was to understand the chemistry education in North Korea and provide it as basic data of chemistry education to prepare for unification of Korean Peninsula.

Poster Presentation : **EDU.P-499**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Elementary school teachers' and preservice elementary teachers' actual and preferred types of science assessment

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In this study, we investigated elementary school teachers' and preservice elementary teachers' actual and preferred types of science assessment with focus on the purpose and the method of assessment. Participants were 75 elementary school teachers and 94 preservice elementary teachers. We administered a questionnaire asking teachers and/or preservice teachers about the types of science assessment they have actually used or would use in future. Teachers' and/or preservice teachers' preferred types of science assessment for hypothetical situations that have been generally reported as the prototypical examples of constructivist science assessment were also examined. The analysis of the actually implemented assessments revealed that most elementary school teachers tended to aim at summative assessment, and that multiple-choice, constructed response, experiment, report, and observation were the prevailing assessment methods. More preservice elementary teachers tended to aim formative assessment and showed preference to experiment and portfolio in assessment methods. For hypothetical assessment situations, both elementary school teachers and preservice elementary teachers exhibited their preferences for various types of constructivist assessment methods, whereas their purposes of the assessment still remained to be traditional.

Poster Presentation : **EDU.P-500**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

Analysis of the reading materials in the chemistry domain of elementary school science and middle school science textbooks and chemistry I and chemistry II textbooks

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In this study, the characteristics of the reading materials in the chemistry domain of elementary school science and middle school science textbooks and chemistry I and chemistry II textbooks developed under the 2009 Revised National Science Curriculum were investigated. The criteria for classifying the reading materials were the types of theme, purpose, presentation and students' activity. The inscriptions in the reading materials were also analyzed from the viewpoint of type, role, caption type, and proximity type. The results indicated that more reading materials were included in the elementary science textbooks than middle school science, chemistry I, and/or chemistry II textbooks. The percentage of 'application in everyday life' theme was high in the reading materials of elementary science textbooks, whereas the percentage of 'scientific knowledge' theme was high in those of middle school science, chemistry I, and/or chemistry II textbooks. It was also found that the percentage of 'expanding concepts' purpose was high in the reading materials of elementary science textbooks, whereas the percentage of 'supplementing concepts' purpose was high in those of middle school science, chemistry I, and/or chemistry II textbooks. Several limitations in the use of inscriptions were found to exist; most inscriptions were photograph and/or illustration; many inscriptions were presented without a caption; there was a problem in the proximity of inscriptions to text.

Poster Presentation : **EDU.P-501**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

A Case Study of Pre-service Secondary Science Teachers' Lessons Using Analogies

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In this case study, we investigated the lessons using analogies conducted by pre-service secondary science teachers. Four pre-service teachers at a college of education in Seoul participated in this study. During teaching practicum, they conducted lessons using analogies. All of the teaching-learning materials were collected, and their lessons were observed and videotaped. Semi-structured interviews were also conducted before and after their lessons. For the analyses, we used a revised framework from previous works which characterized the dimensions of teaching through analogies.

The analyses of the results revealed that the pre-service teachers used pre-planned analogies in most cases. When they used improvised analogies, however, they used analogies unsystematically. They also used analogies once in a lesson, and they thought using analogies repeatedly could make students confused. Although they used student-centered activities such as the role-playing analogy activity, they explained and analyzed analogies. They did not explicate mapping because they thought mapping was so obvious that students could understand mapping. Although they covered the differences between analogues and target concepts, they dismissed simple differences and placed much value upon fancy differences. There were some cases that they confused analogies with examples. Educational implications of these findings are discussed.

Poster Presentation : **EDU.P-502**

Chemistry Education

Grand Ballroom, THU 11:00~12:30

An Analysis of the PCK Components of Middle School Science Teacher's Guidebooks Developed Under the 2009 Revised National Curriculum

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In this study, we investigated the characteristics of the PCK components in the chemistry units of middle school science teacher's guidebooks developed under the 2009 Revised National Curriculum. The analysis of the results revealed that the sub-components of topic-specific strategies, vertical articulation, and lesson objectives were systematically handled in most teacher's guidebooks. However, subject-specific strategies, assessment methods, and curricular changes were mainly dealt with only in the general guidelines. Experiments and inquiries, assessment questions, and assessment dimensions were lack of constructivist approaches in the aspect of presented contents or forms. Horizontal articulation and knowledge of students were either lacked in relevant content or presented in the form of simple presentation. Concepts and theories accounted for the largest proportion of teachers' guidebooks, but some of them were beyond appropriate levels. On the bases of the results, the implications for the development of the teacher's guidebooks are discussed.

Poster Presentation : **ENVR.P-503**

Environmental Energy

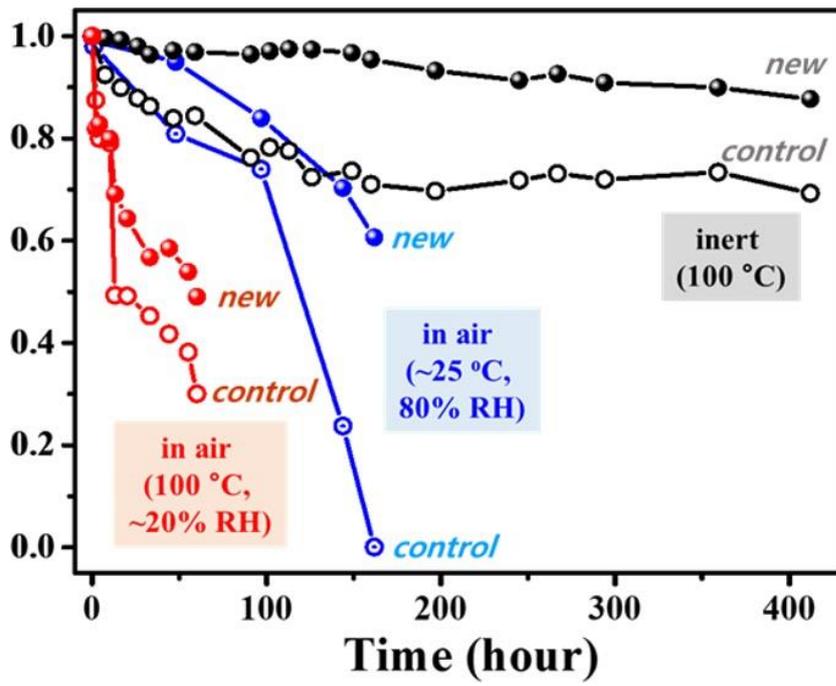
Grand Ballroom, THU 11:00~12:30

Inorganic-organic double layer for efficient hole transport and improve stability in perovskite solar cells

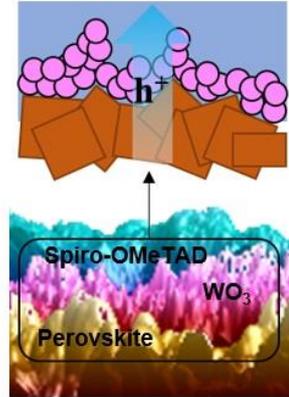
Guan-Woo Kim, Junwoo Lee, Taiho Park*

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

Perovskite solar cells (PSCs) have reached their highest efficiency with 2,2',7,7'-tetrakis(N,N'-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD). However, this material can cause problems with respect to reproducibility and stability. Herein, we report a solution-processable inorganic-organic double layer based on tungsten oxide (WO₃) and spiro-OMeTAD as a hole transport layer in PSCs. The device equipped with a WO₃/spiro-OMeTAD layer achieves the highest efficiency (21.44%) in the tin (IV) oxide planar structure. The electronic property of the double layer is thoroughly analyzed using photoluminescence, space-charge-limited current, and electrochemical impedance spectroscopy. The WO₃/spiro-OMeTAD layer exhibits better hole extraction ability and faster hole mobility. The WO₃ layer particularly improves the open-circuit voltage (VOC) by lowering the quasi-Fermi energy level for holes and reducing charge recombination, resulting in high VOC (1.17 V in the champion cell). In addition, the WO₃ layer as a scaffold layer promotes the formation of a uniform and pinhole-free spiro-OMeTAD overlayer in the WO₃/spiro-OMeTAD layer. High stability under thermal and humid conditions stems from this property. Our study presents a facile approach for improving the efficiency and stability of PSCs by stacking an organic layer on an inorganic layer.



P-type WO_3
Porous scaffold
Uniform, Compact,
Pinhole-free HTL



Poster Presentation : **ENVR.P-504**

Environmental Energy

Grand Ballroom, THU 11:00~12:30

Ultrathin few-layer MoS₂ nanosheets supported on graphene nanofoam towards flexible micro-supercapacitors

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Molybdenum disulfide (MoS₂) is regarded as a representative layered two-dimensional (2D) material in energy storage, and attracting considerable attention for energy storage devices. In this work, simple and scalable fabrication of ultrathin few-layer MoS₂ nanosheets supported on graphene nanofoam (GNF) is developed by combining a straightforward solvothermal method to synthesize an ultrathin MoS₂ and graphene nanofoam made from chemical vapor deposition (CVD). Transfer of MoS₂/GNF onto flexible substrate allows a highly efficient fabrication of mSCs with unique flexibility, mechanical stability, and potential application in wearable electronics. The as prepared MoS₂/GNF mSC exhibit an outstanding electrochemical performance in terms of high volumetric capacitance and capacitance retention after 10,000 cycles. The MoS₂/GNF mSC exhibit simultaneously ultrahigh energy density and power density in a H₃PO₄ gel polymer electrolyte.

Poster Presentation : **ENVR.P-505**

Environmental Energy

Grand Ballroom, THU 11:00~12:30

Low temperature processable perovskite solar cell based on SnO₂ nanoparticle and polyelectrolytes

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Organic-inorganic mixed halide perovskite solar cell (PSCs) have been studied in recent years due to their superior optical, electrical properties, such as long charge diffusion lengths, panchromatic absorption, solution processability, a sharp optical bandgap, abundance of ingredients and very high absorption coefficient. To date, significant research efforts have been devoted in PSCs and a power conversion efficiency (PCE) have reached to 23% in less than five years. Recently, various studies have been carried out to achieve the remarkable progress of PSCs, for example, interface engineering, additives, solvent engineering, compositional engineering and diffusion engineering. Among various approaches, interfacial engineering has attracted considerable interest as effective and simple method for improving device performance. In this work, we employed the two well-known polyelectrolytes (PEs) including amine group on their side chain as cathode buffer layer in planar heterojunction solar cells: Poly[9,9-dioctyl-9',9'-bis[3-(trimethylammonio)propyl][2,2'-bi-9H-fluorene]-7,7'-diyl bromide (PFN-Br) and Polyethylenimine ethoxylated (PEIE). For planar perovskite solar cells, we fabricated the solar cells with the device architecture of glass / ITO / SnO₂ / PEs / perovskite / Spiro-MeOTAD / MoO₃ / Ag. Furthermore, we investigated the effect of two different PEs on the morphology, bandgap tuning and performance of perovskite solar cells. Finally, due to the interaction between SnO₂ and the amine groups on the side chains of the both PEs, we could obtain the better device performance.

Poster Presentation : **ENVR.P-506**

Environmental Energy

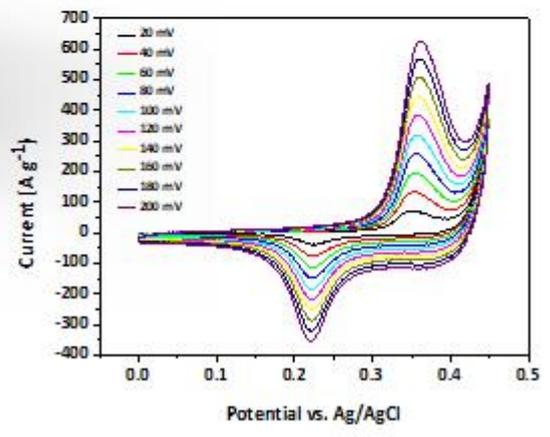
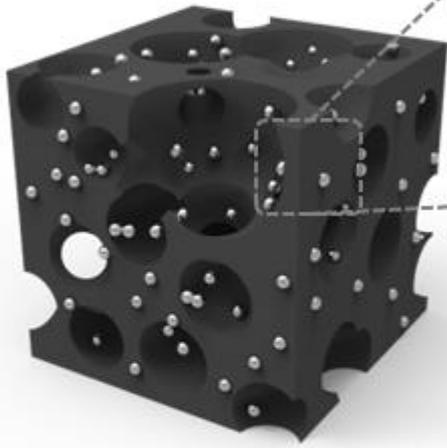
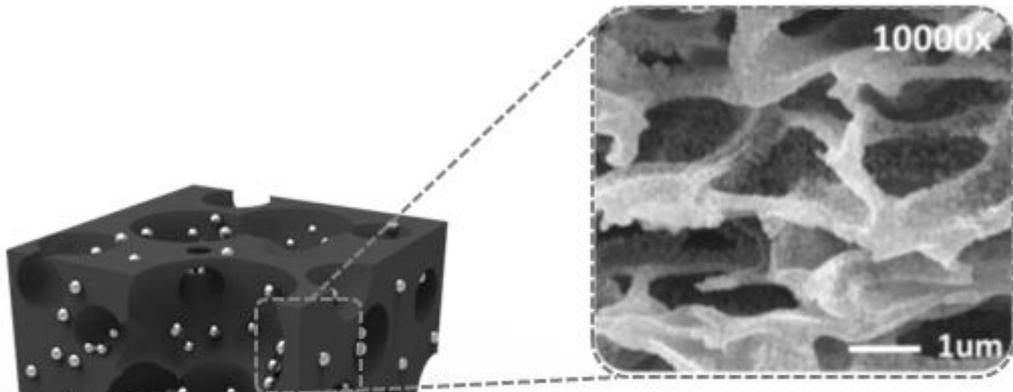
Grand Ballroom, THU 11:00~12:30

Metal Hydroxide Nanoparticles Doped Porous Carbon as High Performance Supercapacitor Electrodes

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Nowadays, electrochemical energy storage and conversion (EESC) devices have been rapidly developed due to an increase in demand for portable electronic equipment and electric vehicles. Among various EESC devices, supercapacitor, which shows high power density and cycle stability, is a strong candidate for high power applications. Porous carbon material is one of the most widely used for supercapacitor electrodes because of its high electric conductivity, high surface area and controllable porosity.[1] However, since porous carbon based supercapacitors store energy through surface charge separation at the electrode/electrolyte interface, it shows relatively low capacitance and energy density. Therefore, metal oxides or hydroxides are added onto the porous carbon in order to increase capacitance and energy density with reversible faradaic redox reactions occurring at the electrode surface.[2, 3] Herein, we report various metal hydroxide nanoparticles (e.g. Ni, Co, Fe) deposited onto nitrogen-doped porous carbon as high performance supercapacitor electrodes (2572.1 F/g at 100mC for Ni). Nitrogen-doped porous carbon has high electric conductivity (3200 S·m⁻¹), high surface area (442.83 m²g⁻¹), high ion diffusion rate and enhanced wettability (contact angle 19.65°). Also, uniformly distributed metal hydroxide nanoparticles on the surfaces of nitrogen-doped porous carbon can facilitate fast intercalation and deintercalation of charges.[3] Therefore, our electrodes for supercapacitor developed in this work have a potential for high performance which can possibly be applied to various wearable energy storage devices. References 1. S. Lee, G. Kim, J. Kim, D. Kim, D. Lee, H. Han and J. Kim, Accepted in Adv. Sustainable Syst. (2018). 2. Y. Liu, N. Fu, G. Zhang, M. Xu, W. Lu, L. Zhou and H. Huang, Adv. Funct. Mater. 27, 1605307 (2017). 3. H. Li, Y. Gao, C. Wang, G. Yang, Adv. Energy Mater. 5, 1401767 (2015).



Poster Presentation : **ENVR.P-507**

Environmental Energy

Grand Ballroom, THU 11:00~12:30

CFD Modeling of the Effect of Bubble Two Bubble Sizes on Bubble-Particle Interaction Rate in a Column for Deinking

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Paper recycling is important due to economic and environmental reasons. Removal of ink from waster paper is necessary to obtain proper pulps for production of recycled paper. Waste paper can be paper from books, newspapers, or other printed material. Removal of ink can be achieved by froth flotation using an agitated tank or an aerated column. It has been reported that big bubble sizes are not beneficial to float fine particles. Ink particles can be agglomerated using reagents. The ink particles are hydrophobic and have a wide range of sizes, from 1-1000 μm . In this work, ink particles of diameter of 60 μm with a contact angle of 30 degrees were used in CFD modeling. The particles had a density of 2600 kg/m^3 , were monosized, and their concentration was 1% v/v. Two air bubble diameters of constant size were modeled, relatively large bubbles of 5 mm and small bubbles of 1 mm. The air injection was 7 l/min. Drag and turbulent dispersion forces and gravity were considered. Flotation kinetics consisted of three processes of bubble-particle interaction, which are collision, attachment and detachment. Each process was represented as probabilities and taking in account turbulence. The results showed that the number of attached particles increased as bubble size decreased. In fact, when bubbles of 5 mm diameter were used, the flotation was only 10% measured as fraction of floated particles after 320 seconds of flotation. Fine particles tend to avoid collision by following liquid streamlines around a rising bubble, especially for large bubbles. In addition, net attachment rates inside the column are higher when the bubble size is small. Therefore, flotation in aerated columns can be improved by reducing bubble size, as well as including mixing. **This research was supported by the Korea Energy and Mineral Resources Engineering Program (KEMREP). **References[1] Chaiarekij, S., H. Dhingra, and B. V. Ramarao. "Deinking of recycled pulps using column flotation: energy and environmental benefits." *Resources, conservation and recycling* 28.3-4 (2000): 219-226.[2] Beneventi, D., et al. "Hydrodynamics and recovered papers deinking in an ozone flotation column." *Chemical Engineering and Processing: Process Intensification* 48.11-12 (2009): 1517-1526.[3] Vashisth, Subhashini, et al. "Column Flotation Deinking: State-of-the-art and opportunities." *Resources, Conservation and Recycling*

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Poster Presentation : **ENVR.P-508**

Environmental Energy

Grand Ballroom, THU 11:00~12:30

Conjugated polyene-functionalized graphitic carbon nitride with enhanced photocatalytic water-splitting efficiency

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Photocatalytic water splitting has attracted the interest from lots of researcher due to its potential application for ready to shortage of natural resource. A graphitic carbon nitride (g-C₃N₄) is one of the promising photocatalyst and advantages of this material is non-metal based, eco-friend, visible light absorption and easy-approach for sythesis. However, fast recombination rate, slow carrier movement in photocatalyst and durability are still remain as challenges inhibiting photocatalytic hydrogen production. Herein, a g-C₃N₄/conjugated polyene (CP) complex is synthesized through a simple calcination method. The g-C₃N₄/CP complex showed photocatalytic activity of lower photoluminescence intensity, higher photocurrent density and finally increase of hydrogen production rate. We investigated the role of CP and found that it help the charge separation form g-C₃N₄ as well as prevent the degradation of photocatalyst during reaction. The best photocatalytic hydrogen production rate of g-C₃N₄/CP is 1270 $\mu\text{molg}^{-1}\text{h}^{-1}$ under visible light ($420 \geq \lambda$), while the g-C₃N₄ is 810 $\mu\text{molg}^{-1}\text{h}^{-1}$. The g-C₃N₄/CP complex prepared 340 °C exhibits better activity than those at 240 and 400 °C. We suggest the simple and cost-effective way to prepare non-metal photocatalyst with high photocatalytic activity and hope to be contribute to this area.

Poster Presentation : **ENVR.P-509**

Environmental Energy

Grand Ballroom, THU 11:00~12:30

Study on Biodegradation of Toxic Organic Contaminants by a microbial fuel cell

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This study was aimed at exploring biodegradation of toxic organic contaminants in wastewater by MFC technology. Toxic organic contaminants: “BTEX (benzene, toluene, ethyl benzene and xylene)”, chloroform and chlorobenzene with concentration from 12.5 ppm to 50 ppm were used as the sole carbon sources in MFCs. Removal efficiencies and electrochemical properties were evaluated in order to explore the feasibility and efficiency of biodegrading toxic organic contaminants and generating electricity simultaneously. Maximum cell voltage of 0.21 V was obtained while using chlorobenzene as sole carbon source. Maximum removal efficiency of 100 % was obtained while benzene was used as a sole carbon source, and maximum power density of 115 mW m⁻², 84 mW m⁻², 94 mW m⁻², 89 mW m⁻², 107 mW m⁻², and 68 mW m⁻² were obtained using ‘BTEX’, chloroform and chlorobenzene as the sole carbon sources, respectively.