

Plenary Lecture : **PLEN-1**

Plenary Lecture

Convention Hall 1+2, THU 13:30

Chair: Sang-Won Lee (Korea University)

High Resolution Ion Separations, Reaction, and Storage; Towards a Flexible Gas Phase Ion Chemistry Workbench based upon Structures for Lossless Ion Manipulations

Richard D Smith

Biological Sciences Division, Pacific Northwest National Laboratory, United States

Gas phase ion chemistry is of broad interest and has importance in areas ranging from fundamental physics, to analytical chemistry, to biomedical research, and most of its applications are done in conjunction with the use of mass spectrometry (MS). New MS applications as well as related instrumental platform advances increasingly involve ion manipulations that are conducted between the ion source and MS analyzer. These manipulations include: ion transport through regions of elevated pressure, ion trapping, reactions (both ion-molecule and ion-ion), and ion mobility (IM)-based separations. While performing these manipulations can extend measurement capabilities or provide new kinds of information, the practicality of such manipulations becomes increasingly constrained by the cost and inefficiency of conventional instrumental designs and ion optic approaches as their complexity or the number of manipulation steps involved increases. For example, advances in MS-based analytical applications are often limited by their speed in conjunction with the use of liquid chromatography separations. In this regard, IM separations provide additional separation power and the basis for more sensitive, complete and effective analyses, as well as additional structure-related information (i.e., collision cross sections) that can be derived from these separations. The benefits of IM separations increase as separation power increases, and the limitations on both its resolving power and sensitivity have constrained applications of IM with MS.

To address these challenges, we are developing new approaches for ion manipulations based upon effectively lossless RF confinement achieved in readily fabricated Structures for Lossless Ion Manipulations (SLIM). An important aspect of these developments has been the use of traveling waves to drive and control ion motion in conjunction with SLIM. This has allowed the development of compact long separation path length (serpentine) designs that enable much higher resolution IM separations than

previously feasible. The use of traveling waves in SLIM has also enabled a host of new capabilities. This includes the creation of extremely large ion trapping volumes and the ability in both spatially and temporally to compress ion populations, including IM separations, without loss of resolution.

This presentation will describe the basis for SLIM as well as recent developments that address many current challenges within a range of applications and that provide new capabilities, such as the basis for a broadly flexible ion chemistry workbench.



Award Lecture : **AWARD-1**

Award Lecture

Convention Hall 3, FRI 13:30

Chair: Sang-gi Lee (Ewha Womans University)

Development of New Synthetic Methods in Organic Synthesis

Phil Ho Lee

Department of Chemistry, Kangwon National University, Korea

In this award lecture, a variety of synthetic methods that have been developed over the last 30 years from my laboratory will be introduced. First, alkyl, alkenyl, alkynyl, allyl, allenyl, and acyl cross-coupling reactions using a wide range of in situ generated organoindium reagents will be presented. On the basis of Au-catalyzed hydrophosphoryloxylation, the synthetic methods for novel phosphaheterocyclic compounds have been developed through C–H activation using phosphoryl directing groups. Also, my research focuses on developing new synthetic approaches for heterocyclic compounds using diazo compounds, triazoles, pyridotriazoles, and thiadiazoles in the presence of transition metal catalysts. Recently, my laboratory is interested in selectively activating B–H bond in carboranes and understanding reactivity of nonbenzenoid aromatic compounds.

Symposium : **POLY1-1**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403, THU 15:40

Chair: Myung-Han Yoon (GIST)

Stimuli-Responsive Polymers with Tunable Sensitivity Driven by Morphological Change for Sensing Applications

Hyung-il Lee

Department of Chemistry, University of Ulsan, Korea

In this presentation, the thermo/photo-tunable detection of mercury (II) ions by polymeric micelles based on thermo/light-responsive block copolymers will be discussed. Even though the thermo/light-induced disruption of micelles has many applications, such as drug deliveries in which the photocontrolled release of the encapsulated drugs is possible, it has been rarely studied for the sensing applications. To the best of our knowledge, the current work presented in talk is the first example of the thermo/light-triggered turn-on colorimetric detection of mercury (II) ions by light-responsive block copolymer micelles. No detection of mercury (II) ions was observed initially, but micellar disruption by light irradiation resulted in turn-on detection. The general strategy presented herein can potentially be used for the preparation of polymeric micelles capable of the thermo/light-induced tunable detection of various kinds of water-soluble analytes.

Symposium : **POLY1-2**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403, THU 16:10

Chair: Myung-Han Yoon (GIST)

Formation of organic semiconducting crystalline wires for the application to polymer-gated organic devices

Seungmoon Pyo

Department of Chemistry, Konkuk University, Korea

The performance organic/polymer based electronic devices such as light-emitting diodes, thin-film transistor, and non-volatile memory device have been improved recently, and some of them have been reached to the level of commercialization. But, the development and formation technology of active component of the organic devices are still very critical issue. In this presentation, a formation of highly-ordered organic semiconducting crystalline wire and its application to organic electronic devices will be discussed. A few types of active layers composed of n- and p-type organic semiconductor, an organic micro crystal embedded layer and laterally stacked organic crystal, will be presented. The devices with the active layer exhibit selective charge transport characteristics varying from unipolar to ambipolar depending on the composition of the active layer. We also present the formation and analysis of the short channel device for high speed operation using the organic semiconducting crystalline wire.

Symposium : **POLY1-3**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403, THU 16:40

Chair: Myung-Han Yoon (GIST)

Imaging Behavior of Highly Fluorinated Materials under Electron-Beam and Extreme UV Radiation

Jin-kyun Lee

Department of Polymer Science & Engineering, Inha University, Korea

In this presentation, I propose a new concept of organic small molecule-based extreme UV (EUV) resist materials that do not require sub-stoichiometric ingredients. Based on the previous results with highly fluorinated electron-beam resists, it was possible to design amorphous small molecules equipped with perfluoroalkyl ether chains. The synthesis of the prototype was carried out successfully, and its physical properties, imaging mechanism, and performance were all evaluated under electron beam exposure conditions. Although the prototype showed slightly low sensitivity to EUV irradiation, I was able to mitigate the issue by appending other cross-linkable functional moieties. The modified version showed decent negative-tone patterning performance under e-beam exposure and could form images under EUV irradiation and the pattern development step using highly fluorinated solvents.

Symposium : **POLY1-4**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403, THU 17:10

Chair: Myung-Han Yoon (GIST)

Semiconducting Polymers Consisting of New Donating and Accepting Building Blocks for Organic Photovoltaic Cells

Do-Hoon Hwang

Department of Chemistry, Pusan National University, Korea

Organic photovoltaic (OPV) cells based on a polymer/fullerene bulk-heterojunction (BHJ) active layer have emerged as promising, next-generation energy sources arising from their attractive properties: flexibility, low weight, and potential for low-cost, high-throughput manufacturing. Considerable efforts to develop new materials, device architectures, and processing techniques, have led to dramatic improvements in power conversion efficiencies (PCEs). One of the most important issues for enhancing the power conversion efficiency (PCE) of organic photovoltaic cells (OPVs) has been the development of π -conjugated polymers that exhibit broad visible wavelength absorption, high charge carrier mobility, suitable energy level matching of frontier orbitals with those of the electron acceptor, and appropriate chain orientation that form an optimum pathway for the charge carriers to the electrodes. In this presentation, I will talk about recent progress on new donor-acceptor type conjugated polymers for organic photovoltaic cells conducted in our research lab.

Symposium : **POLY2-1**

Recent Trends in Polymer Synthesis

Room 403, FRI 09:00

Chair: Myungeun Seo (KAIST)

Thiourea-based Aromatic Gels: Anion-Responsive Soft Actuator and Sensor

Changsik Song

Department of Chemistry, Sungkyunkwan University, Korea

Anion-coordination chemistry have played important roles in biology and industrial processes, in addition to environmental issues. Thiourea has been studied for the tailored anion receptors via hydrogen bonding interactions, but seldom applied to anion-responsive actuators. In this study, we prepared thiourea-based soft gels using a facile one-step synthesis and tested for anion-specific or anion-selective responses in actuation (i.e., volume transition). Thiourea-based soft gels showed visually considerable color changes depending on the anions' basicity (e.g., highly basic F⁻ and CN⁻). But remarkably different size changes were observed for F⁻ (contraction) and CN⁻ (expansion). We investigated anion-specific effects, similar to Hofmeister effects in water, and found that the interesting volume changes were due to the interplay of anions' basicity, solvation energy and accompanying osmosis. Finally, such properties were utilized as anion-responsive soft actuators.

Symposium : **POLY2-2**

Recent Trends in Polymer Synthesis

Room 403, FRI 09:25

Chair: Myungeun Seo (KAIST)

Polymers and Polymerization for Coating Living Cells

Sung Ho Yang

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

Cytocompatible coating of living cells have drawn a great attention with aims of useful methods for protecting inner cells, providing chemical functionality on cell surfaces, and controlling cell proliferations. The first attempt of living cells coating has been conducted by organic polymers through layer-by-layer methods. The impact of works was under-evaluated in the biomedical fields because the method was limited to microbial cells and the macromolecular coating had no particular roles. To achieve more practical demonstration, coating materials shifted from organic polymers to inorganic materials, in other words, from soft to hard materials such as silica, titania, calcium carbonate, and calcium phosphate. The toughness of the inorganic materials were beneficial for protecting the cells and controlling cell division. In these works, the polymers have been used as catalytic templates for biomimetic synthesis of inorganic materials. On the other hand, it was developed a cytocompatible surface-initiated, atom transfer radical polymerization (SI-ATRP) method for grafting polymers from living cells with use of polydopamine priming. Considering a plethora of functional and structural variations in synthetic polymers, grafting polymers from (or to) cell surfaces would generate multifunctional cellular hybrids for many biotechnological and biomedical applications, not to mention providing an advanced tool for chemically manipulating the cells.

Symposium : **POLY2-3**

Recent Trends in Polymer Synthesis

Room 403, FRI 10:00

Chair: Myungeun Seo (KAIST)

Influence of Material Properties on Scratch-Healing Performance of Intrinsic Self-healing Polymers

Jin chul Kim

Center for Green Fine Chemicals, Korea Research Institute of Chemical Technology, Korea

Polymer coatings have been used to protect substrate surfaces from the external environment and/or to enhance aesthetic appearance. Recently, however, polymer coats have evolved to perform various 'smart' functions such as self-healing, self-cleaning, and stimulus-response functions. Intrinsic self-healing coatings are among the most important technologies for the use of high-value products that require long-term mechanical stability and chemical resistance, as required in automotive, architectural, medical, and electronic devices. The advantages of this approach over the extrinsic scratch-healing technique are that it can be applied to a wide range of organic coating materials, it can be used with transparent coatings, it allows the repeatedly healing of scratches. Overall, however, the durability of the coating is inversely related to its scratch-healing performance because the former requires high crosslinking density, while the latter relies on enhanced polymer chain mobility so that polymer chain rearrangements and hence healing can occur more easily. Therefore, striking the right balance between the material properties and the self-healing performance is a key factor in designing high-performance scratch-healing coating materials. In the current study, we conducted a detailed investigation of the relationship between the material properties and scratch-healing performance of intrinsic self-healing polymers containing diverse dynamic covalent bonds.

Symposium : **POLY2-4**

Recent Trends in Polymer Synthesis

Room 403, FRI 10:25

Chair: Myungeun Seo (KAIST)

Epoxy-Based Copolymers: A Simple, But Versatile Toolbox for Functional Material Platforms

Myungwoong Kim

Department of Chemistry, Inha University, Korea

Epoxy containing polymeric materials have been of great importance in academy and industries due to its applicability toward a variety of functional materials. Specifically, its ability to form crosslinked structure has been exploited in various applications. Herein, we describe simple, versatile, efficient and readily scalable chemical routes using epoxy-based copolymers to achieve complex polymeric structures exhibiting desired chemical functionalities. As proof of concept, we show three different structures: polymer brush thin films, particles with unconventional morphologies, and nanofiber mats. Those structures were effectively fabricated with epoxy-based polymers, and the surface functionalities were controlled with simple and efficient chemistries such as nucleophilic addition and thiol based click chemistries. The ease of synthesis, chemical tunability, and stability highlight effectiveness of the copolymers as a versatile toolbox to impart desirable functionalities to create various functionalized interfaces in soft materials.

Symposium : **POLY3-1**

Polymer Development for Energy & Environment

Room 403, FRI 14:30

Chair: Han Young Woo (Korea University)

Molecular Orientation-Dependent Photovoltaic Performance in Organic Solar Cells

Kilwon Cho

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

Photovoltaic performance of organic solar cells is highly dependent on the anisotropic nature of optoelectronic properties of photoactive materials. Here, we demonstrate an approach for highly efficient planar heterojunction solar cells by tuning the molecular orientation of the organic semiconducting materials. Face-on orientation of donor materials led to enhanced optoelectronic properties including light absorption, exciton diffusion, charge transport, and interfacial energetics. Enhanced exciton separation at the face-on donor-acceptor interface was observed as well. These results imply that the molecular orientation in photoactive layers is a critical factor that should be elaborately controlled for future high performance organic solar cells.

Symposium : **POLY3-2**

Polymer Development for Energy & Environment

Room 403, FRI 15:00

Chair: Han Young Woo (Korea University)

Highly Efficient, Photostable Ternary Organic Solar Cells Using Narrow Bandgap Nonfullerene Acceptor and Fullerene Additive

Kwanghee Lee

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

Recent breakthroughs in the molecular design and the device engineering in the field of nonfullerene acceptor (NFA)-based organic solar cells (OSCs) have made remarkable achievement with high power conversion efficiencies (PCEs) over 17%. However, despite such promising advances, an inferior stability of OSCs under operational conditions (e.g., light and heat) is a prominent challenge that must be overcome for their practical commercialization. Recently, a ternary blend concept has been suggested to be an efficient way to simultaneously enhance the PCE and the stability of OSCs. Here, by introducing small amount of fullerene into narrow bandgap NFA-based bulk heterojunction nanocomposites, we developed efficient and photostable ternary photoactive systems, leading to the enhanced PCE of 13% and the prolonged lifetime that retained about 80% of their initial PCEs after 500 hr operation under continuous illumination, whereas binary counterparts underwent rapid degradation. It appears that the fullerene additive provides an excellent compatibility for efficient electron transfer and balanced charge transport with suppressed recombination.

Symposium : **POLY3-3**

Polymer Development for Energy & Environment

Room 403, FRI 15:30

Chair: Han Young Woo (Korea University)

Conducting polymers and their application to highly stable and green processable hybride solar cells with high efficiency

Taiho Park

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

Perovskite solar cells (PSCs) have attracted much attention owing to their high power conversion efficiencies (PCEs) and relatively low fabrication costs compared with conventional silicon-based solar cells. In a planar n-i-p-type PSC, a perovskite layer is sandwiched between a fluorine-doped tin oxide (FTO) glass substrate with an electron transport layer (ETL) and a hole transport layer (HTL) with metal electrode, respectively. Great efforts have been made to improve power conversion efficiency, but less attention are in their stability. In this talk, I would like to discuss how we improve stability of perovskite solar cells with high performance.

Symposium : **POLY3-4**

Polymer Development for Energy & Environment

Room 403, FRI 16:00

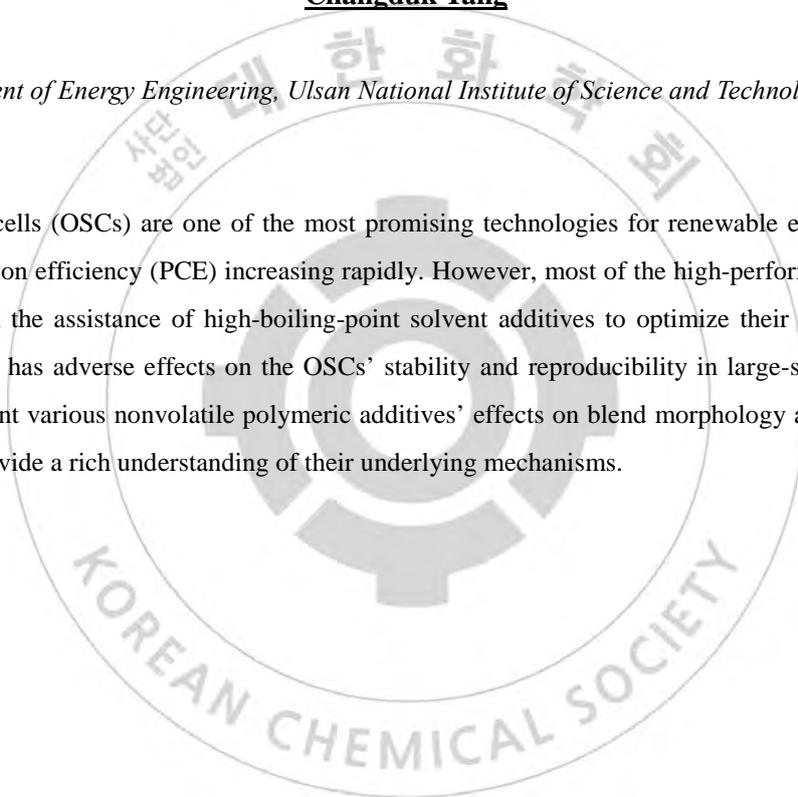
Chair: Han Young Woo (Korea University)

Application of Nonvolatile Polymeric Additives in Organic Solar Cells

Changduk Yang

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

Organic solar cells (OSCs) are one of the most promising technologies for renewable energy with their power conversion efficiency (PCE) increasing rapidly. However, most of the high-performance OSCs are fabricated with the assistance of high-boiling-point solvent additives to optimize their charge transport properties; this has adverse effects on the OSCs' stability and reproducibility in large-scale production. Here, we present various nonvolatile polymeric additives' effects on blend morphology and performance of OSCs to provide a rich understanding of their underlying mechanisms.



Symposium : **INOR1-1**

Recent Trends in Metal-Organic Frameworks

Room 401+402, THU 15:40

Chair: Nak Cheon Jeong (DGIST)

Symmetry-Guided Syntheses of Mixed-Linker Zr-MOFs with Precise Linker Locations

Myoung Soo Lah

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

The construction of multifunctional mixed-linker metal-organic frameworks (MOFs) with precise linker locations in the framework is a challenging task. A series of new Zr-MOFs with 12-c fcu topology containing the two linkers with different linker symmetries and lengths at well-defined locations are prepared. While one-pot reactions of zirconium metal ion with mixtures of dicarboxylate heterolinkers result in only hybrid Zr-MOFs with fcu topology, symmetry-guided stepwise reactions produce a series of Zr-MOFs with fcu topology containing two different dicarboxylate linkers with precise locations in the framework. The symmetry-guided insertions of linear terephthalic acid (H₂BDC) derivatives with mmm symmetry into the mmm symmetry-sites of the flexible 8-c bcu Zr-MOF (termed ZRN-bcu) composed of zigzag 2,6-naphthalenedicarboxylic acid with 2/m symmetry result in a series of new Zr-MOFs with 12-c fcu topology. Even though the length of the BDC₂- derivatives is much shorter than the distance between the unlinked closest neighboring Zr-clusters in ZRN-bcu, the symmetry-matching BDC₂ derivatives are induced-fit into the framework of ZRN-bcu to form a series of stable 12-c fcu Zr-MOFs containing two different dicarboxylate linkers at well-defined locations.

Symposium : **INOR1-2**

Recent Trends in Metal-Organic Frameworks

Room 401+402, THU 16:10

Chair: Nak Cheon Jeong (DGIST)

Toward Novel and Versatile Building Block for Zr-based Prototype MOFs

Hyungphil Chun

Department of Applied Chemistry, Hanyang University, Korea

Recent market-oriented developments for metal-organic frameworks (MOFs) ask for simple, easy-to-prepare and stable MOFs which are surprisingly rare among tens of thousands of systems known in literatures. Therefore, it has been sought to discover a new prototype MOF that could readily be expanded into a series of simple and stable crystalline porous materials. In particular, Zr-carboxylate systems with simple ligands have been targeted by varying solvothermal reaction conditions. It has been found out that inorganic acids are potentially good substitutes for commonly used monocarboxylic acid modulator. This presentation introduces some results obtained by this approach, namely formate-based [Zr₃₆] macrocycles and MOF-like framework. Ongoing efforts toward non-carboxylate Zr building blocks will also be included.

Symposium : **INOR1-3**

Recent Trends in Metal-Organic Frameworks

Room 401+402, THU 16:30

Chair: Nak Cheon Jeong (DGIST)

Catalysis in nanostructured materials for energy-conversion

Seok Min Yoon

Department of Chemistry, Wonkwang University, Korea

Nanostructured materials are highly suitable as electrocatalyst and photocatalyst supports in electrochemical energy conversion and solar energy conversion devices. The intrinsic performance of catalysts is affected by their intrinsic nanostructure, comprising nanoscopic building blocks whose properties can be altered by factors such as mechanical stresses, electric fields, magnetic fields, light irradiation and so on. Such materials are often discovered by serendipity but it would be highly desirable to design them in rational ways to achieve what can be termed as "Functionality by Design". The catalytic capability requires development of various synthetic approaches and thorough understanding of physico-chemical properties across several length-scales – from individual nanocomponents all the way to macroscopic nanostructured materials. In my talk, I will discuss such rational strategies applied to catalytic materials from zero- to three-dimensional and having hybrid architectures comprising nanoparticles as well as metal organic frameworks. I will illustrate the applications of such nanostructured in electrocatalysis in metal-air batteries, and in photocatalysis for water purification and potentially for artificial photosynthesis. In particular, the large single crystal MOFs we study exhibit bifunctional electrocatalytic behavior by supporting efficient and stable oxygen reduction reaction (ORR) close to the direct four-electron process, and oxygen evolution reaction (OER). This ORR/OER bifunctionality allows our MOF-based batteries to efficiently use humid air (i.e., oxygen and water) as "fuel". Overall, the combination of these effects with aluminum anode translates into battery's remarkable discharge capacity.

Symposium : **INOR1-4**

Recent Trends in Metal-Organic Frameworks

Room 401+402, THU 17:00

Chair: Chang Yeon Lee (Incheon National University)

New Approaches of Metal-Organic Frameworks toward Hydrogen Isotope Separation

Hoi Ri Moon

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

Metal-organic frameworks (MOFs) have attracted great attention in gas storage and separation over the past decades, owing to their high level of porosity and chemical and structural tunability. Recent increase in global demand for isotopic gases, particularly deuterium, have triggered the researches to separate physico-chemically almost identical isotopic mixture with MOFs by tuning the pore size or introducing open metal sites (OMSs) as strong binding site. Nonetheless, the difficulty of optimizing the pore size to the sub-Angstrom scale and insufficient separation efficiency of OMSs limits the synthesis of MOFs with high deuterium-selectivity. Therefore, there is a critical need for new approaches utilizing MOFs in hydrogen isotope separation. In this talk, we present two novel strategies toward well-designed MOF-based separation systems that can effectively separate deuterium from hydrogen isotopic mixture. The first strategy exploits the dynamic pore change during the breathing of a flexible MOF, MIL-53(Al), for the high selectivity for D₂ over H₂. During the flexible and reversible transition, the pore apertures are continuously adjusted, thus providing the tremendous opportunity to separate mixtures of similar-sized and similar-shaped molecules that require precise pore tuning. The other strategy is the simple post-modification of introducing imidazole molecules into the highly dense OMS channels of MOF-74 to optimize the aperture size and increase the internal binding energy, simultaneously. It can synergistically maximize the efficiency of deuterium separation, having a high uptake with the highest reported separation factor as high as ~26 at 77 K. We believe that our results will provide new opportunities for the intelligent design of porous materials leading to the development of other highly efficient isotope and gas separation systems.

Symposium : **INOR1-5**

Recent Trends in Metal-Organic Frameworks

Room 401+402, THU 17:20

Chair: Chang Yeon Lee (Incheon National University)

Investigation of Reaction Sites on Metal-Organic Frameworks-Based Catalysts

Min Kim^{*}, Nakcheol Jeong^{1,*}

Department of Chemistry, Chungbuk National University, Korea

¹*Department of Chemistry, Korea University, Korea*

The investigation of the reaction site is important when MOF (metal-organic framework)-based heterogeneous catalysts are employed, *i.e.*, whether it is inside the crystals or on their surface. Especially, in the case of chiral MOF, the environment of reaction sites for stereoselectivity would vary according to their location. The comparison of reaction efficiency with substrate size has been widely used in discussions on this issue. If there is a threshold point where the reaction rate sharply decreased as the substrate size increased, the reaction of substrates up to that point in size is regarded as having proceeded inside the MOF channels. However, this interpretation should be carefully employed to determine and identify the reaction site in a MOF crystal. In this presentation, a series of reactions will be compared to investigate and identify the reaction sites. Both Zn-mediated stoichiometric carbonyl-ene reaction and Ti-catalyzed carbonyl-ene reaction were individually performed and compared in homogeneous and heterogeneous media with substrate size controls. In the stoichiometric reaction (by Zn), it was clearly demonstrated that the whole MOF crystal is working and the inside of pore is important part for stereoselectivity. However, if the reaction is catalytic (by Ti), it would mainly take place on the surface of the crystals, regardless of the substrate size. The detail comparison data along with particle size control experiments and two-photon microscopy images will be discussed.

Symposium : **INOR2-1**

Recent Trends in Organometallic Chemistry

Room 401+402, FRI 09:00

Chair: Myung Hwan Park (Chungbuk National University)

***Ortho*-Carbazole-Appended Triarylboron Compounds: From Color Tunable TADF Emitters to Time-Resolved Fluorescence Sensors**

Min Hyung Lee

Department of Chemistry, University of Ulsan, Korea

Triarylboron compounds have attracted great interest in the fields of optoelectronic applications, such as anion sensors and OLEDs, due to their high Lewis acidity and excellent photophysical properties. Recently, our group first demonstrated that *ortho*-donor-appended triarylboron compounds can function as highly efficient TADF (thermally activated delayed fluorescence) emitters in OLEDs due to twisted donor-acceptor structure and strong electron-accepting properties of triarylboron moiety. To generalize this concept and to further develop color-tunable TADF emitters, we have prepared a series of *ortho*-carbazole-appended triarylboron compounds, where the substituted carbazolyl unit acts as a donor (D) and substituted triarylboron as an acceptor (A), respectively. Various electron-donating and/or -accepting groups were employed in the donor and acceptor units of the reference Cz_oB compound, which allowed for full emission color tuning in the visible region. Furthermore, TADF properties of these compounds were successfully applied to the design of time-resolved turn-on fluorescence sensor for hydrogen peroxide (H₂O₂). Details of synthesis and properties of triarylboron compounds will be discussed.

Symposium : **INOR2-2**

Recent Trends in Organometallic Chemistry

Room 401+402, FRI 09:20

Chair: Myung Hwan Park (Chungbuk National University)

Strategic Molecular-Design for High Chemical-Stability of Blue Phosphors in OLEDs

Kang Mun Lee

Department of Chemistry, Kangwon National University, Korea

Organic electroluminescent devices (OLEDs) were first reported by Tang and VanSlyke in 1987. They have since received a great deal of scientific, industrial, and commercial attention because of their latent capabilities, such as excellent brightness, fast response time, low turn-on voltage, and wide viewing angle, which make them suitable to use as full-colour displays and flexible light sources. In order to ensure the high quantum efficiency of full-colour organic light-emitting diode (OLED) devices, it is essential to develop phosphorescent luminophores that emit pure red, green, and blue colours with high electrochemical stability and radiative efficiency. Although several Ir(III)-cyclometalates that exhibit pure red and green phosphorescence with excellent performance, markedly high efficiency, and long lifetime have been developed for use in OLEDs, it is necessary to introduce further improvements in the quantum efficiency and lifetime of OLED devices based on blue phosphorescent luminophores, which currently show relatively poorer chemical and electrochemical properties due to their intrinsic wide band gap. In this presentation, specific strategy for enhancing high chemical-stability of blue phosphores, which can be applicable to commercialization in OLEDs, will be shown. In addition, systematically designed and synthesized two phenyl-imidazole-moiety-based iridium complexes will be presented as an example, which can lead to an increased energy band-gap and enhanced blue emissive performance, especially long device lifetime.

Symposium : **INOR2-3**

Recent Trends in Organometallic Chemistry

Room 401+402, FRI 09:40

Chair: Myung Hwan Park (Chungbuk National University)

Imidazo[1,5-a]pyridine-derived N-Heterocyclic Carbene Ligands

Sukwon Hong

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

N-heterocyclic carbene (NHC) has emerged as an important ligand in homogeneous catalysis. Imidazo[1,5-a]pyridin-3-ylidene (ImPy) ligands are a rigid bicyclic variant of N-heterocyclic carbenes. ImPy ligands are strong sigma donors as a result of the extended pi-system. Substituents on the bicyclic ImPy can be projected into the metal coordination sphere, often resulting in bonding interactions with the metal center. Synthesis of ImPy precursors is concise and allows late-stage incorporation of diverse functional substituents. We envision that ImPy ligands will provide a versatile framework where a various functional group can be easily implemented to create the optimal electronic and steric environment for catalysis. Several transition metal complexes containing ImPy ligands have been prepared. The ImPy-Cu complexes efficiently catalyzed the direct C-H carboxylation of benzoxazole with CO₂. ImPy-Ni catalysts exhibited catalytic activity in acrylate synthesis from ethylene and CO₂. ImPy-Ru catalysts exhibited good reactivity in ethenolysis of methyl oleate. Current progress on ImPy transition metal catalysts will be discussed in details in the presentation.

Symposium : **INOR2-4**

Recent Trends in Organometallic Chemistry

Room 401+402, FRI 10:10

Chair: Kang Mun Lee (Kangwon National University)

Transition-Metal-Catalyzed Decarboxylative Coupling Reactions

Sunwoo Lee

Department of Chemistry, Chonnam National University, Korea

Transition-metal-catalyzed decarboxylative coupling of alkynoic acids have been studied by our lab for a decade. Since our first report that palladium-catalyzed reactions of aryl halides and propiolic acids afforded the symmetrical and unsymmetrical diaryl alkynes in good yields, a variety of related methodology have been reported by many research groups including us. 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. Although the decarboxylative coupling of alkynoic acids and Sonogashira type coupling of terminal alkyne showed similar reactivity in most cases, the unique reactivity of alkynoic acid has been found. It is noteworthy that arylpropiolic acids readily prepared from the coupling reaction of aryl halides and propiolic acid without column chromatography procedure. In this presentation, we would like to discuss some of our recent research progress towards the decarboxylative coupling reactions of alkynoic acids. The synthesis of alkynyl ketone, propargyl amine, allyl nitrile and multi-halogenated compounds will be presented.

Symposium : **INOR2-5**

Recent Trends in Organometallic Chemistry

Room 401+402, FRI 10:30

Chair: Kang Mun Lee (Kangwon National University)

Development of Metal Precursors and Application to ALD/CVD

Taek-Mo Chung

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

We have focused on the development of novel precursors for atomic layer deposition (ALD) and chemical vapor deposition (CVD) for a few decades. To synthesize the desired metal precursors, we adopted the synthetic strategy for the design of organic ligands on the molecular level. From the research works, various organic ligands such as aminoalkoxides and N-alkoxy carboxamides have been synthesized and applied to prepared new metal precursors which exhibit high volatility and thermal stability and are suitable to be applied to thin films deposition by ALD/CVD. They are nickel, copper, ruthenium, and strontium precursors for their applications in memory devices. In addition, new metal precursors such as tin, indium, and gallium complexes have been recently developed for transparent conducting oxides (TCO) and applied to deposit their oxide thin films such as SnO, SnO₂, In₂O₃, and InZnSnO_x by ALD and CVD. In this presentation, we will discuss development and application of new metal precursors for ALD/CVD.

Symposium : **INOR3-1**

Recent Trends in Supramolecular Chemistry

Room 305+306, FRI 14:30

Chair: Junseong Lee (Chonnam National University)

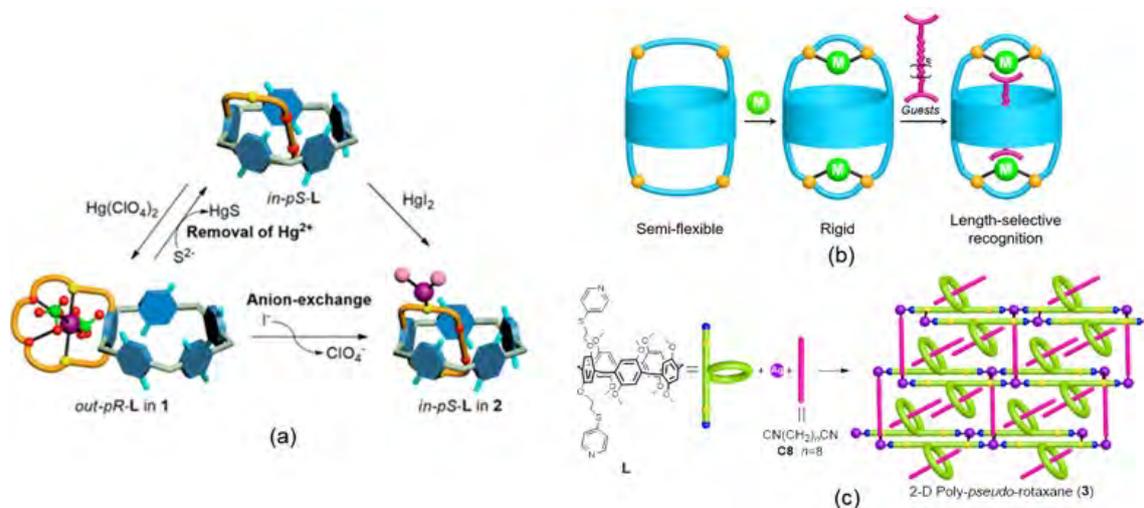
Pillar[5]arenes, Invitation to Metallosupramolecular Chemistry: Metal-Induced Chiral Inversion, Adaptive Guest Binding, and Polypseudorotaxane

Shim Sung Lee

Department of Chemistry, Gyeongsang National University, Korea

Pillar[n]arenes are new macrocyclic host and their organic guest-based supramolecular chemistry has been extensively studied.¹ However, their coordination compounds are very rare due to large cavity and lack of metallation site. Recently, we have proposed bicyclic,² tricyclic,³ and armed⁴ pillararenes as new build blocks for constructing metallosupramolecules. First, we synthesized a bicyclic pillar[5]thiacrown (*rac-L*) and resolved its enantiomers (*in-pS-L* and *in-pR-L*) (Fig. a).² The *in-pS-L* recognizes Hg²⁺ to trigger the chiral inversion to *out-pR-L*, and it takes place in the presence of ClO₄⁻ or NO₃⁻. The crystallographic approach reveals that the anions act as coordination mode-directing species which play a decisive role on the chiral inversion. Second, the tricyclic pillar[5]-bis-dithiacrown shows the dimetalation via two crown subunits and then uptakes CN(CH₂)₂CN selectively over analogous dinitrile guests with different lengths (Fig. b).³ This is a chemical example of the adaptive guest binding of biological receptors which are rigidified by metalation to recognise substrates precisely. Third, one-pot reaction of a thiopyridyl pillar[5]arene (**L**) with silver(I) trifluoroacetate in the presence of a linear dinitrile guest **C8**, [CN(CH₂)_nCN, n=8], afforded the first example of a 2-D polypseudorotaxane {[Ag(**L**)(**C8**)_{1.5}]CF₃CO₂]_n whose guest **C8** not only threads into the pillararene unit but also crosslinks the parallel coordinative polymeric arrays (Fig. c).⁴ The formation of the 2-D polypseudorotaxane is driven by adaptive rearrangement of the 1-D backbone to minimize the repulsion between threading **C8** and steric complementarity on crosslinking. A formation pathway of the 2-D polypseudorotaxane is proposed. The above works demonstrate a new perspective on metallosupramolecules of pillararenes. **References** 1. Ogoshi, T.; Kanai, S.; Fujinami, S.; Yamagishi, T.-a.; Nakamoto, Y. *J. Am. Chem. Soc.* **2008**, *130*, 5022. 2. Lee, E.; Ju, H.; Kuwahara, S.; Ikeda, M.; Habata, Y.; Lee, S. S. *J. Am. Chem. Soc.* **2018**, *140*, 9669. 3. Lee, E.; Ryu, H.; Ju, H.; Kim, S.; Lee, J.-E.; Jung, J. H.;

Kuwahara, S.; Ikeda, M.; Habata, Y.; Lee, S. S. *Chem. Eur. J.* **2019**, *25*, 949-4. Lee, E.; Ju, J.; Kim, S.; Jung, J. H.; Habata, Y.; Lee, S. S. *In preparation*.



Symposium : **INOR3-2**

Recent Trends in Supramolecular Chemistry

Room 305+306, FRI 15:00

Chair: Junseong Lee (Chonnam National University)

Reversible Structural Flexibility of Pd₆L₈ Cages via Recognition of Alkyl Sulfate Surfactants

Ok-Sang Jung*, Dongwon Kim¹

Department of Chemistry, Pusan National University, Korea

¹*Pusan National University, Korea*

A new strategy for inner-cavity control of coordination cages using various alkyl sulfates as a molecular glue has been carried out. Self-assembly of palladium(II) nitrate with new tridentate 1,3,5-tris(4-nicotinamide-phenoxy)benzene (L) produces [Pd₆L₈]¹²⁺ cages with the inner cavity of 19 × 21 × 25 Å³. The addition of alkyl sulfates (ROSO₃⁻, R = ethyl-, octyl-, decyl-, dodecyl-, and tetradecyl-) produces a host-guest interaction assembly, inducing the cavity contraction of the coordination cages with the inner cavity of 13 × 13 × 13 Å³. This cage specifically binds to the sulfate moiety via hydrogen bonds between O of the sulfate and H of the amide, enabling the cage to recognize the alkyl length of the alkyl sulfates. The contact angles of a drop of liquid on the surface of crystalline solid are strongly depending on the alkyl chain length of the included alkyl sulfates.

Symposium : **INOR3-3**

Recent Trends in Supramolecular Chemistry

Room 305+306, FRI 15:40

Chair: Junseong Lee (Chonnam National University)

Self-assembly of BODIPY based Metal Supramolecules: Synthesis and Applications

Chang Yeon Lee

Department of Energy and Chemical Engineering, Incheon National University, Korea

Coordination-driven self-assembly process remains one of the most convenient technique to design complicated yet interesting large metal based supramolecules with well-defined architectures.¹ The size, shape, geometry and overall properties can be fine-tuned by proper selection of appropriate electron-deficient metal-nodes and electron-donor multidentate ligands. Since the initial findings on palladium and platinum macrocycles in the early 1990s by Fujita et. al., Stang and Cao, macrocycles based on other metal centers have attracted substantial interest in different important fields of chemistry.² Following a similar strategy, Therrien et. al. synthesized ruthenium-based rectangles, prisms, and cubes with excellent biological properties.³ My research group in Incheon National University, introduced the use of highly fluorescent pyridyl-BODIPY (boron-dipyrromethene) ligands to develop novel metal-based supramolecules.⁴ In this talk, I will present the recent progress of metal-based BODIPY supramolecules evolved from our research group and their applications in cancer therapy.⁵References:(1)T. R. Cook, Y.-R. Zheng, P. J. Stang, Chem. Rev. 2013, 113, 734-777.(2) (a) M. Fujita, J. Yazaki, K. Ogura, J. Am. Chem. Soc. 1990, 112, 5645-5647; (b) P. J. Stang, D. H. Cao, J. Am. Chem. Soc. 1994, 116, 4981-4982. (3)B. Therrien, CrystEngComm. 2015, 17, 484-491.(4)C. Y. Lee, O. K. Farha, B. J. Hong, A. A. Sarjeant, S. T. Nguyen, J. T. Hupp, J. Am. Chem. Soc. 2011, 133, 15858-15861.(5)(a) G. Gupta, A. Das, N. B. Ghate, T. Kim, J. Y. Ryu, J. Lee, N. Mandal, C. Y. Lee, Chem. Commun. 2016, 52, 4274-4277; (b) G. Gupta, A. Das, S. Panja, J. Y. Ryu, J. Lee, N. Mandal, C. Y. Lee, Chem. Eur. J. 2017, 23, 17199-17203; (c) G. Gupta, A. Das, K. C. Park, A. Tron, H. Kim, J. Mun, N. Mandal, K.-W. Chi, C. Y. Lee, Inorg. Chem. 2017, 56, 4615-4621.

Symposium : **INOR3-4**

Recent Trends in Supramolecular Chemistry

Room 305+306, FRI 16:00

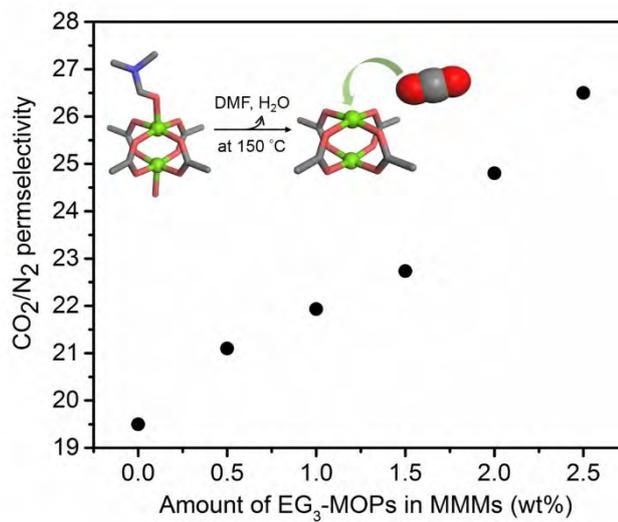
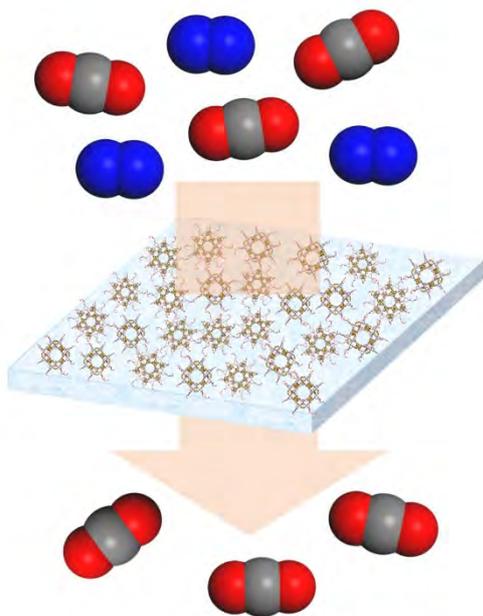
Chair: Junseong Lee (Chonnam National University)

Mixed-Matrix Membranes with Hydrophilic Metal-Organic Polyhedra for Efficient CO₂ Separation

Hyunuk Kim

Energy Materials Laboratory, Korea Institute of Energy Research, Korea

Defect-free mixed-matrix membranes (MMMs) were prepared by incorporating hydrophilic metal-organic polyhedra (MOPs) into cross-linked polyethylene oxide (XLPEO) for efficient CO₂ separation. Hydrophilic MOPs with triethylene glycol pendant groups, which were assembled by 5-tri(ethylene glycol) monomethyl ether isophthalic acid and Cu(II) ions, were uniformly dispersed in XLPEO without particle agglomeration. Comparing with conventional neat XLPEO, the homogenous dispersion of EG₃-MOPs in XLPEO enhanced CO₂ permeability of MMMs. Upon increasing the amount of EG₃-MOPs, the membrane performance such as CO₂/N₂ selectivity was steadily improved because of unsaturated Cu(II) sites at paddle-wheel units, which was confirmed by Cu K-edge XANES and TPD analysis. Therefore, such defect-free MMMs with unsaturated metal sites would contribute to enhance CO₂ separation performance.



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

Current Advances in Reaction Dynamics

Room 305+306, THU 15:40

Chair: Yoonsoo Pang (GIST)

Circular dichroism spectroscopy of chiral molecules and ions in the isolated gas phase

Nam Joon Kim

Department of Chemistry, Chungbuk National University, Korea

CD spectra measured in solution represent only the average CD values of all conformational isomers. In contrast, the CD spectroscopy of molecules or ions in the isolated gas phase can provide conformation-selective CD values without influence of solvent molecules. We have developed an efficient CD spectroscopic technique that can be used to measure the CD spectra of cold chiral molecules and ions in the gas phase. Using this CD technique, we investigated the induced circular dichroism (ICD) phenomena of jet-cooled chiral complexes. Although CD is generally observed for chiral molecules, achiral molecules can have CD when they are bound with a chiral molecule through noncovalent interactions, which is denoted as ICD. ICD has been extensively employed to investigate the structures and binding properties of various host-guest complexes. We obtained the first isomer-selective ICD spectra of jet-cooled phenol complexes with (-)-methyl L-lactate (PhOH-(-)ML). The ICD values of the two conformers have different signs and magnitudes, which were explained by differences both in the geometrical asymmetries of PhOH bound to (-)ML and in the electronic coupling strengths between PhOH and (-)ML. Comparing the ICD values of various PhOH complexes with other chiral molecules, we identified the physical properties that might govern the differences in their ICD values. Recently, we have also developed a new technique to measure the CD spectra of molecular ions produced by electrospray ionization using cryogenic cold ion spectroscopy. We will discuss the potential application of this technique to larger biomolecular systems.

Symposium : **PHYS1-2**

Current Advances in Reaction Dynamics

Room 305+306, THU 16:10

Chair: Yoonsoo Pang (GIST)

Molecular reaction dynamics by time-resolved wave packet spectroscopies and molecular dynamics simulation

Wooseok Heo, Junwoo Kim¹, Taiha Joo*

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

¹Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science, Korea

For a photochemical reaction occurring in an electronic excited state, one powerful way to study the molecular reaction dynamics is to record the nuclear wave packet motions following the photoexcitation to the Franck-Condon state. Evolution of the wave packets may contain extensive information on the potential energy surfaces (PES) and reaction coordinates. We have performed time-domain experiments such as pump-probe transient absorption (TA) and time-resolved fluorescence (TF) with high enough time resolution to record the nuclear wave packet motions of the reactant and product. We have also devised a way to distinguish between the vibrational modes that are orthogonal to the reaction coordinate and those that are coupled strongly to the reaction from the molecular dynamics simulation. Combining the experiment and theory, one can achieve a detailed picture of the molecular reaction dynamics. We demonstrate the strength of this approach by applying to the excited state intramolecular proton transfer (ESIPT) reactions 10-hydroxybenzo[h]quinoline (HBQ) and its derivatives.

Symposium : **PHYS1-3**

Current Advances in Reaction Dynamics

Room 305+306, THU 16:35

Chair: Yoonsoo Pang (GIST)

Ionic effects on excited state proton transfer reaction of Coumarin 183 in aqueous ionic solutions

Joonyoung F. Joung, Sangin Kim, Sungnam Park*

Department of Chemistry, Korea University, Korea

A photoacid is an aromatic compound that has a lower pKa in its electronic excited state than its ground state and has been used as a model system to study the excited-state proton transfer (ESPT) reactions and proton transfer processes. Although proton dissociation (PD) reactions of weak acids and proton transfer (PT) processes in aqueous solutions are strongly influenced by dissolved ions, a detailed molecular picture that describes how ions affect the rates of PD and PT processes is still missing. Here, we utilize time-resolved fluorescence spectroscopy combined with density functional theory (DFT) calculations to investigate the ionic effect on the ESPT reaction of Coumarin 183 (C183) in aqueous ionic solutions. The local hydrogen bond structure of C183 in the ionic hydration shell is strongly influenced by cations. The activation energy for the ESPT of C183 increases as the charge density of cations is increased. Most importantly, quantum chemical calculations indicate that the proton's positive charge in the transition state is delocalized through a hydrogen-bonded water channel and is more destabilized as the charge density of cations is increased, leading to a higher activation energy for the ESPT. Finally, the ionic effects on the equilibrium (pKa and pKa*) and kinetic (Ea and KIE) parameters of C183 are found to be well-explained by the free-energy reactivity relation. Our experimental and DFT calculation results provide a molecular level understanding of cationic effects on the equilibria and ESPT kinetics of photoacids in aqueous ionic solutions.

Symposium : **PHYS1-4**

Current Advances in Reaction Dynamics

Room 305+306, THU 17:10

Chair: Hyungjun Kim (KAIST)

Photochemistry based on excited state molecular dynamics

Seung Kyu Min

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

Reaction dynamics on electronic excited states plays an important role in photochemical/physical phenomena such as photosynthesis, vision process, and artificial light harvesting. Due to high complexity of topology in excited state potential energy surfaces, theoretical/computational description of excited state molecular dynamics is crucial to understand those phenomena. The most popular computational tool for excited state molecular dynamics is trajectory surface hopping (TSH) algorithm even though TSH has a serious drawback known as the lack of quantum decoherence. Here I introduce a novel method for excited state molecular dynamics, so-called decoherence-induced surface hopping based on exact factorization (DISH-XF), which can handle electron-nuclear correlation and quantum decoherence correctly with minimal computational costs. Moreover, I provide several applications of DISH-XF method including nonadiabatic electrons transfer, photodissociation, light-induced ring opening, cis-trans photoisomerization, and light-induced molecular rotary motors.

Symposium : **PHYS1-5**

Current Advances in Reaction Dynamics

Room 305+306, THU 17:35

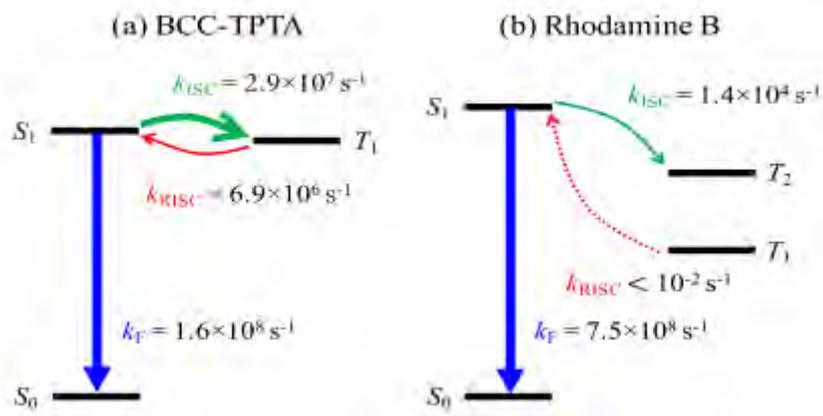
Chair: Hyungjun Kim (KAIST)

Ultra-Fast Spectroscopy to Probe the Excited State Dynamics of Reported Highly Efficient Thermally Activated Delayed Fluorescence Chromophore

Hyungjun Kim

Department of Chemistry, Incheon National University, Korea

Multiple ultrafast spectroscopic techniques and quantum chemical simulations (QCS) were used to investigate the excited state dynamics of BCC-TPTA. This organic chromophore is believed to possess excited state dynamics governed by a thermally activated delayed fluorescence (TADF) mechanism with a reported internal quantum efficiency of 84 %. In addition, a significant enhancement in its quantum yield in solution after purging oxygen has been reported. This enhancement has been widely accepted as due to a delayed fluorescence process occurring in the μ s time-scale. The spectroscopic measurements were carried out both in solution and blended films, and from fs to μ s time-scales. The excited state dynamics of Rhodamine B and Ir(BT)₂(acac) were also probed for comparison. Investigations in the absence of oxygen were also carried out. Our time-correlated single photon counting (TCSPC) measurements revealed a lack of long-lived emissive lifetime for BCC-TPTA in any of the medium tested. Our ns transient absorption spectroscopy (ns TAS) experiments revealed that BCC-TPTA does not possess triplet transient states that could be linked to a delayed fluorescence process. Instead, the evidence obtained from our spectroscopic tools suggests that BCC-TPTA has excited state dynamics that of a typical fluorescence chromophore and that just comparing the quantum yield difference before and after purging oxygen from the solution is not an accurate method to claim excited state dynamics governed by a delayed fluorescence mechanism. Consequently, we believe that previous studies, in which the photo-physics of organic chromophores with TADF characteristics are reported, may have overlooked the influence of the host materials on the obtained optical properties in blended films.



Symposium : **PHYS2-1**

Current Advances in Theoretical and Computational Chemistry

Room 305+306, FRI 09:00

Chair: Changsun Eun (Hankuk University of Foreign Studies)

CASPT2 photochemistry

Jae Woo Park

Department of Chemistry, Chungbuk National University, Korea

Second-order complete active space perturbation theory (CASPT2) is one of the most efficient *ab initio* methods toward accurate descriptions of both static and dynamical electronic correlations. Here, I will talk about recent progress in CASPT2 to calculate excited states potential energy surfaces and the surface crossings between excited states and the ground state. In particular, the automatic code generation technique has been used to simplify and implement tensor operations in the CASPT2 formalism. With these developments, locating conical intersections of molecules with >50 atoms and performing molecular dynamics simulations with >20 atoms are now routine. I will also discuss some practical issues of the MRPT calculations for calculating excited states, such as selections of zeroth-order Hamiltonian and level shifts.

Symposium : **PHYS2-2**

Current Advances in Theoretical and Computational Chemistry

Room 305+306, FRI 09:20

Chair: Changsun Eun (Hankuk University of Foreign Studies)

DFT studies on size-dependent level alignment between anatase and rutile TiO₂ nanoparticles

Kyoung Chul Ko

Department of Chemistry Education, Chonnam National University, Korea

It is well known that conventional local-density approximation (LDA) and generalized gradient approximation (GGA) based functionals severely underestimate the band gap of oxides including TiO₂ materials. The broadly used hybrid functionals such as PBE0 and B3LYP give too large calculated band gap values for TiO₂. To avoid so-called band gap problem in DFT and to describe the electronic structure of TiO₂ materials properly, we proposed a modified hybrid functional containing 12.5 % of non-local Fock exchange called as PBEx [1]. Based on this PBEx functional, the prediction of size dependent band alignment in anatase and rutile nanoparticles was investigated [2]. A predictive map of how the anatase-rutile level alignment varies from the smallest nanoparticles to the bulk was provided on the basis of vacuum-referenced electronic levels. In agreement with most recent works, a staggered type II anatase level alignment is predicted for the bulk, which we further find to persist into the regime of large NPs. Our results also suggest that other level alignments which are less favorable for photocatalysis will emerge when the diameter of the TiO₂ NPs is reduced below ~15 nm. References [1] Kyoung Chul Ko, Oriol Lamiel-Garcia, Jin Yong Lee, and Francesc Illas, *Phys. Chem. Chem. Phys.* 18, 12357 (2016) [2] Kyoung Chul Ko, Stefan T. Bromley, Jin Yong Lee, and Francesc Illas, *J. Phys Chem. Lett.* 8, 5593 (2017)

Symposium : **PHYS2-3**

Current Advances in Theoretical and Computational Chemistry

Room 305+306, FRI 09:40

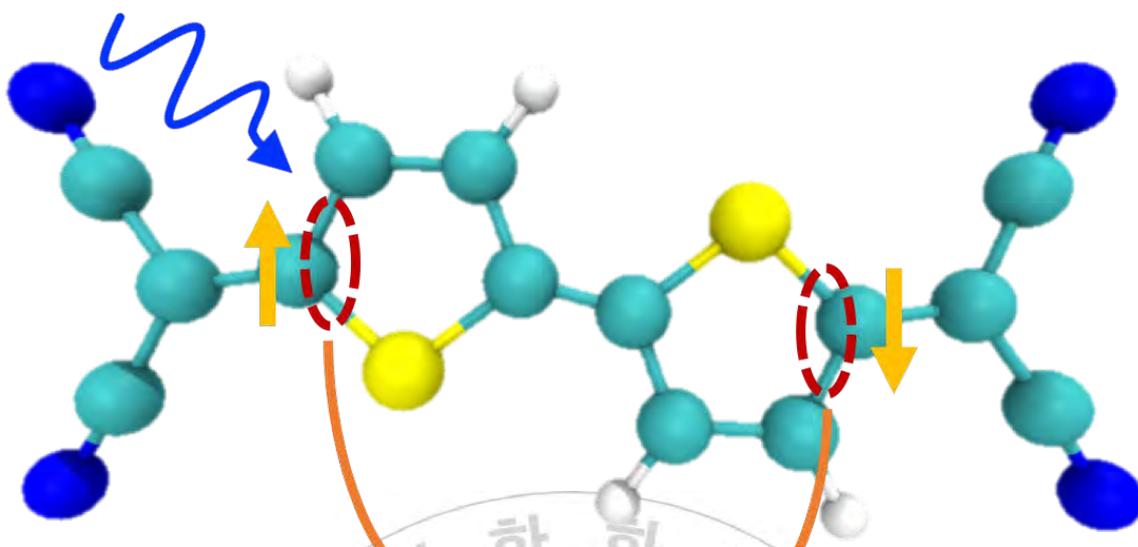
Chair: Changsun Eun (Hankuk University of Foreign Studies)

Enacting Two-Electron Transfer from a Double-Triplet State of Intramolecular Singlet Fission

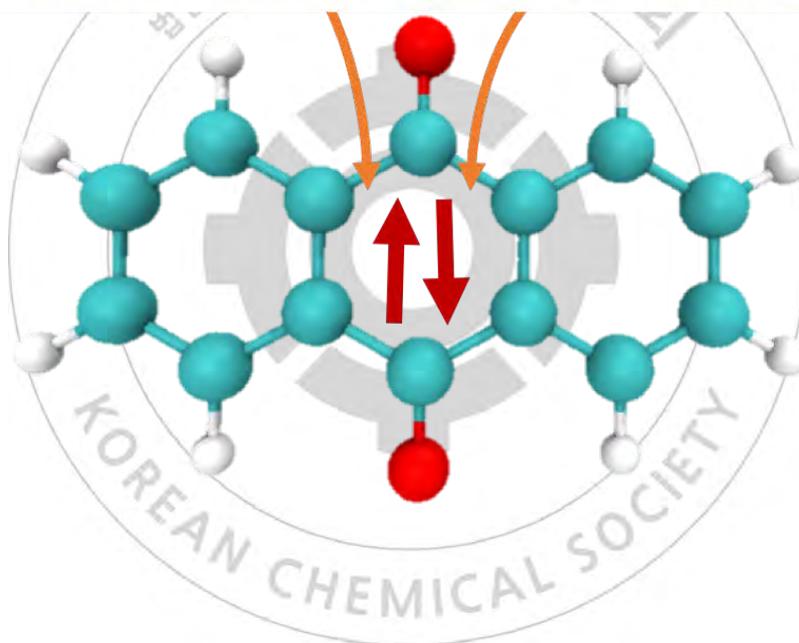
Hyungjun Kim

Department of Chemistry, Incheon National University, Korea

Generating, transferring, and storing multiple electrons from single photons could prove revolutionary for solar energy technologies. One promising process, singlet fission (SF), produces two excited electrons from a single photon.¹ This approach could be useful to overcome the theoretical solar cell's efficiency (Shockley-Queisser limit) and create highly efficient solar cells by reducing thermally wasted high-energy photons. More than one electron needs to be transferred to realize the improvement of photovoltaic cells. In this talk, I will present a simulation-led strategy enacting two-electron transfer between an intramolecular singlet fission chromophore (tetracyanomethylene quinoidal bithiophene with β, β' -solubilizing groups) and multielectron acceptor (anthraquinone).² The thermodynamic plausibility of multielectron transfer from a double-triplet state and the absorption spectra of electron transfer (ET) products were predicted using quantum chemical simulations. These predictions are consistent with experimental observations of reduced lifetimes in time-resolved fluorescence spectroscopy, changes in transmission profile, and appearance of new absorption bands in transient absorption spectroscopy, all of which support multi-ET in the QOT2/AQ mixture. The analysis suggests 2ET is favored over 1ET by a 2.5:1 ratio.



Multi-Electron Transfer



Symposium : **PHYS2-4**

Current Advances in Theoretical and Computational Chemistry

Room 305+306, FRI 10:00

Chair: Changsun Eun (Hankuk University of Foreign Studies)

Computational studies on functionalization of 2D materials

Jaehoon Jung

Department of Chemistry, University of Ulsan, Korea

Interfacial interaction has long served as a key element to get fundamental insights into surface science and related chemical phenomena. Understanding interfacial interaction is, therefore, of great importance to achieve robust predictability and high controllability in a variety of applications. Herein we discuss the role of interfacial interaction in the functionalization of 2D materials, which is crucial for applying them as a component in functional device or as a catalyst via tuning their chemical and physical properties. Computational studies based on density functional theory were performed to explain the experimental observation for the hydroxylation of graphene epitaxially grown on metal substrate. The formation of hydroxylated graphene with a highly-ordered fashion, which was observed in scanning tunneling microscopy study, can be understood with interfacial interaction between graphene sheet and underneath metal substrate. In addition, a few on-going studies related to the functionalization of 2D materials will also be introduced in this presentation.

Symposium : **PHYS2-5**

Current Advances in Theoretical and Computational Chemistry

Room 305+306, FRI 10:20

Chair: Changsun Eun (Hankuk University of Foreign Studies)

Computational Approach to Electrocatalytic Reactions using New Theoretical Methodology: One Probe and Non-Equilibrium Surface Green's Function

Sang Uck Lee

Department of Bionano Technology, Hanyang University, Korea

The electrochemical reactions on the surfaces of several catalysts are critical to the development of high performing energy harvesting and storage devices. Therefore, in recent years, many theoretical and experimental studies have been conducted to evaluate the precise catalytic reaction mechanisms and catalytic activity for the development of new catalyst materials. However, the catalytic reaction mechanism has not been clearly defined, even for commonly used Pt catalysts, because all the possible factors that dictate the electrocatalytic reactions have not been yet fully considered. Although the theoretical approach has been improved by considering the kinetic activation energy and explicit electrolyte molecules in the free energy diagram (FED) method proposed by Norskov, all theoretical catalytic reaction studies possess fundamental limitations due to the use of the slab model, which is difficult to consider electron reservoir and external potential. In this work, we used new methodology of one probe and Non-Equilibrium surface Green's Function (OPNS) to overcome the limitations of slab model by coupling the surface to an infinite reservoir of electrons and to properly consider external potential on the electrocatalytic reactions. Especially, we tried to solve the controversy over the iodine reduction reaction (IRR) mechanisms on the Pt(111) surface, consecutive or concerted mechanisms, using OPNS.

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

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 14:30

Chair: Jongwoo Lim (Seoul National University)

Understanding the charging dynamics of an ionic liquid electric double layer capacitor

YounJoon Jung

Division of Chemistry, Seoul National University, Korea

We investigate the charging phenomena of an electric double layer capacitor (EDLC) by conducting both equilibrium and non-equilibrium molecular dynamics (MD) simulations. A graphene electrode and 1-ethyl-3-methylimidazolium thiocyanate ionic liquid were used as a system for the EDLC. We clarify the ionic layer structure and show that an abrupt change of the ionic layers leads to a high differential capacitance of the EDLC. The charging simulations reveal that the charging dynamics of the EDLC is highly dependent on the rearrangement of the ionic layer structure. Particularly, the electrode charge during the charging process is consistent with the perpendicular displacement of ionic liquid molecules. From this property, we analyze the contribution of each molecular ion to the electrode charge stored during charging. Charging of the EDLC is largely dependent on desorption of the co-ions from the electrode rather than the adsorption of the counter-ions. In addition, the contribution of bulk ions to the charge stored in the EDLC is as important as that of ions adjacent to the electrode surface contrary to the conventional viewpoint. From these results, we identify the charging mechanism of the EDLC and discuss the relevance to experimental results. Our findings in the present study are expected to play an important role in designing an efficient EDLC with a novel perspective on the charging of the EDLC.

Symposium : **PHYS3-2**

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 15:00

Chair: Jongwoo Lim (Seoul National University)

Nanometric Water Channels in Water-in-Salts Electrolytes of Li-Ion Battery observed with 2D-IR Spectroscopy.

Kyungwon Kwak^{*}, Minhaeng Cho^{*}

Department of Chemistry, Korea University, Korea

Two-dimensional infrared spectroscopy (2D-IR) and polarization selective pump-probe spectroscopy (IR-PP) has been applied to study various chemical and biological processes with femtosecond time resolution. Recently, our group extends research interest into solvation dynamics in non-aqueous organic electrolyte system used in commercial Li-ion battery of electrolytes as well as in highly concentrated aqueous electrolytes for advanced energy storage system. Electrolytes are ubiquitous and indispensable in all electrochemical devices including electrolytic cells, capacitors, fuel cells, or batteries. Their function is the same in devices for serving as the medium for the ion transport between electrodes. The electrolyte determines how fast the energy could be released by controlling the rate of mass flow within the battery. Thus, it has been suggested that the solvation structures and dynamics of Li ions in liquid electrolyte play an essential role to Li-based battery performance. Lithium ions in highly concentrated aqueous electrolyte used in lithium-ion battery (LIB) shows unexpectedly high ion mobility despite high viscosity of the concentrated electrolyte. Here, carrying out femtosecond IR pump-probe and two-dimensional IR spectroscopy studies, we show that a considerable amount of water even in highly concentrated electrolyte solutions exhibits bulk-like water properties and forms hydrogen-bonding network wire structures with nanometer diameters. Furthermore, time-resolved rotational anisotropy, spectral diffusion dynamics, and molecular dynamics simulations of water indicate the presence of interfacial water on ion aggregate networks that helps reducing electrostatic friction of hydrated lithium ions, resulting in an unexpectedly rapid transport of lithium ions.



Symposium : **PHYS3-3**

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 15:20

Chair: Jongwoo Lim (Seoul National University)

Towards controlling of Li_2O_2 structures for improvement of charging overpotential in lithium-oxygen batteries

Hye Ryung Byon

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

The rechargeable lithium-oxygen (Li-O_2) battery, providing theoretically high specific-energy-density calculated as $\sim 3 \text{ kWh kg}^{-1}_{\text{cell}}$, is a promising future energy storage system. However, the over-potential is considerably severe during charge due to difficulty of Li_2O_2 decomposition ($\text{Li}_2\text{O}_2(\text{s}) \rightarrow 2\text{Li}^+ + \text{O}_2(\text{g}) + 2\text{e}^-$, $E_{\text{rev}} = 2.96 \text{ V vs. Li}^+/\text{Li}$), which is one of the greatest challenges for implementation of practical battery systems. Much effort has been devoted by incorporation of metal oxide promoters and soluble redox mediator. However, these additive materials give rise to more side reactions and require high cost. Here I present the new strategy of Li_2O_2 structural engineering to reduce the charge over-potential. The design of electrode surface can enhance adsorption affinity of O_2 and LiO_2 , which determines morphology and structure of Li_2O_2 . We found that the resulting amorphous Li_2O_2 facilely decomposes in comparison with crystal structure, which is attributed to increased ionic and electronic conductivity of Li_2O_2 .

Symposium : **PHYS3-4**

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 15:40

Chair: Jongwoo Lim (Seoul National University)

Promoting water photooxidation on transparent WO₃ thin films using metal oxide overlayers

Wooyul Kim

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

Tungsten trioxide (WO₃) is widely known as one of the most promising water photo-oxidation materials due to the visible range absorption. However, it has inherent limitation in the formation of peroxy species, stability and recombination of surface defect site. Nowadays it's being gradually overcome by different methods, such as surface passivation, oxygen vacancy control and the chemically and physically deposition of co-catalysts. Here, WO₃ (electrodeposited), Al₂O₃/WO₃, and TiO₂/WO₃ (prepared by atomic layer deposition, ALD) electrodes were employed to investigate the role of the passivation overlayer by using both photoelectrochemical activity and laser flash photolysis measurements for charge carrier dynamic. It shows the different photoelectrochemical results based on passivation materials. In particular, femtosecond to microsecond transient absorption spectroscopy measurements of WO₃, Al₂O₃/WO₃, and TiO₂/WO₃ clearly showed that the ultra-fast pathway in the presence of the Al₂O₃ and TiO₂ overlayer (ca. ps) under applied bias condition whereas the relatively long-trapped holes portion increased with overlayer (ca. s), facilitating water photooxidation. Moreover, we also carefully tuned oxygen vacancy of tungsten oxide from W to WO₃ via WO₂ using high temperature anodization method. Through the potassium contained non-aqueous anodization process, few amount of potassium can stabilize to oxygen vacancies in tungsten oxides. Various application of precise tuned tungsten oxide (e.g., both water oxidation and reduction process, oxygen reduction, etc) will be presented.

Symposium : **PHYS3-5**

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 16:00

Chair: Jongwoo Lim (Seoul National University)

Enhancing long-term photostability of BiVO₄ photoanodes for solar water splitting by tuning electrolyte composition

Dong Ki Lee^{*}, Kyoung-Shin Choi¹

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

¹*Chemistry, University of Wisconsin-Madison, United States*

Solar hydrogen production is an attractive way to harvest solar energy into a storable energy carrier. However, the production cost of solar hydrogen is far from reality. One of viable option is constructing photoelectrochemical water splitting cell using chip materials, which can directly utilize solar-driven electrons into hydrogen evolution reaction. Among oxide-based photoelectrodes, n-type BiVO₄ photoanodes have been widely coupled with chip photovoltaic materials (Si and CH₃NH₃PbI₃) because of its early photocurrent onset potential and favorable valance band position for water oxidation. In this presentation, we will present an alternative strategy to suppress photocorrosion of BiVO₄ photoanodes during photoelectrochemical water oxidation. We found that anodic photocorrosion of BiVO₄ photoanodes involves the loss of V⁵⁺ from the BiVO₄ lattice by dissolution. We demonstrate that the use of a V⁵⁺-saturated electrolyte, which inhibits the photooxidation-coupled dissolution of BiVO₄, can serve as a simple yet effective method to enhance the photostability of BiVO₄ during water oxidation for hundreds hours. The effect of the V⁵⁺ species in the electrolyte on photostability of BiVO₄ and recent strategies to improve photoelectrochemical performances of BiVO₄ will be discussed.

Symposium : **PHYS3-6**

Physical Chemistry Approaches in Energy and Environmental Materials

Room 401+402, FRI 16:20

Chair: Jongwoo Lim (Seoul National University)

A descriptor based approach to find promising catalysts – Methane oxidation on transition-metal surfaces as an example

Jong Suk Yoo

Chemical Engineering, University of Seoul, Korea

In this talk, I would like to discuss how density functional theory and microkinetic modeling can be employed to investigate CH₄ oxidation to CO, CO₂, CH₂O, and CH₃OH on Pd(111) under mildly oxidizing conditions. Although our energetic analysis indicates that the metallic site on Pd(111) is more active than O* and OH* on the Pd surface for C–H bond activation, our microkinetic analysis indicates that the metallic site produces mostly CO, whereas the O* site produces mostly CH₂O. In addition, we show that the product selectivity can change significantly depending on the pressures of the products (CO, CO₂, CH₂O, and CH₃OH). Increasing the product pressures leads to the promotion of CO₂ production, because CO oxidation becomes more active than CH₄ oxidation. We then extend the study to other FCC(111) surfaces by incorporating the linear scaling relations in the mean-field microkinetic model. We find that most transition-metal surfaces cannot effectively activate CH₄ under the reaction conditions employed. We find that the kinetics of CH₄ oxidation to CO, CO₂, CH₂O, and CH₃OH can be described generally as a function of two descriptors, enabling identification of the most promising catalyst surface for selective production of the desired product.

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

Advanced Instrumental Analysis Chemistry for Protein Dynamics Studies

Room 202, THU 17:20

Chair: Youngbok Lee (Hanyang University)

Real-time Hyperpolarized Magnetic Resonance Spectroscopy and Imaging

Youngbok Lee

Department of Bio-Nano Engineering, Department of Chemical and Molecular Engineering, Korea

Magnetic resonance (MR) research is one of the most important analytical tools for chemistry and biological study. It provides not only detailed information on the structure of small molecules and macromolecules, but also on molecular interactions. Because of the inherent low sensitivity of MR, which stems from a small Zeeman splitting of the nuclear spin energy states, a long signal averaging time or a high spin concentration is often required. A variety of methods have been explored to improve the sensitivity of MR. Especially, large signal gains can be obtained by hyperpolarization of the nuclear spins. MR signals of hyperpolarized samples are enhanced by several orders of magnitude when compared to the signals from thermal polarization. Dissolution Dynamic Nuclear Polarization (D-DNP) is a versatile technique capable of polarizing many different nuclei in the solid state at low temperature, and subsequently providing a hyperpolarized liquid sample following a dissolution step. The resulting signal enhancement has made it possible to obtain detailed information in research fields as varied as metabolic imaging or enzyme catalysis. This research aims to extend the applicability of dissolution DNP into new areas of chemistry and biology, which involve studying protein-ligand interactions, real-time kinetic and mechanistic studies for enzyme catalyzed and polymerization reactions, and metabolic imaging for early-stage cancer detection.

Symposium : **ANAL1-1**

Advanced Instrumental Analysis Chemistry for Protein Dynamics Studies

Room 202, THU 15:40

Chair: Youngbok Lee (Hanyang University)

3D structure study of colloidal nanocrystals using liquid phase TEM

Jungwon Park

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

Three dimensional (3D) atomic structures of materials govern the physical and catalytic properties of materials. As the material dimension becomes nanometer-scale, 3D structures of colloidal nanocrystals typically deviate from the lattice structures measured and expected in their bulk counterparts. This is presumably because of the dominance of surface dangling bonds, defects, and dislocations within the volume of nanocrystals. To understand these unique structural features of nanocrystal, a method that can precisely determine the positions of the individual atoms is required. We introduce our experimental efforts using a combination of new techniques including graphene liquid cell for in situ TEM, aberration-corrected TEM, structure analysis algorithm, and 3D strain measurement. We apply it to determine the 3D atomic arrangements of different types of nanocrystals in solution. Our high-resolution 3D density maps and fitted atomic models show crystal structures of individual nanocrystals with structural degeneracies, including single crystalline, polycrystalline, distorted structures, and a dislocation. We also discuss the extent of this new analytical method regarding types and dimensions of materials systems which require unprecedented structural information in native conditions.

Symposium : **ANAL1-2**

Advanced Instrumental Analysis Chemistry for Protein Dynamics Studies

Room 202, THU 16:05

Chair: Youngbok Lee (Hanyang University)

X-ray Studies of Water's Anomalous Properties and Ground-State Protein Dynamics with Free Electron Lasers

Kyung Hwan Kim

Department of Chemistry, POSTECH, Korea

X-ray science has evolved dramatically with the use of X-ray free electron lasers (XFELs) such as LCLS, SACLA, PAL-XFEL, European XFEL, and SwissFEL. They can generate ultrashort X-ray pulses with unprecedented brilliance and coherence, and this has been a breakthrough for many X-ray related techniques on a broad range of scientific disciplines and brought us to investigate many interesting new sciences which was previously not possible. In this talk, two recent X-ray studies about the origin of anomalous properties of water and ground-state protein dynamics with free electron laser facilities will be shown. In the liquid form, water has numerous anomalous properties as compared to other liquids such as density maximum at 4-degree C. As an explanation for these anomalous experimental observations, a hypothetical liquid-liquid transition (LLT) and a liquid-liquid critical point (LLCP) has been proposed but has never been proved experimentally. Recently, we developed a new experimental technique utilizing FELs and found the first experimental evidence of the existence of the Widom line which is supposed to emanate from the LLCP [1-2]. With the FELs which provide coherent beams, a new domain for X-ray diffraction of disordered materials becomes possible which can be used to probe the dynamics of the system on a molecular level. The technique is called X-ray Photon Correlation Spectroscopy (XPCS) (3). While other pump-probe type experiments measure the excited-state dynamics, XPCS is a probe-probe type experiment and thus can investigate the true ground-state equilibrium dynamics of proteins or other materials. Reference [1] K. H. Kim et al., Science, 358, 1589-1593 (2017) [2] K. H. Kim et al., Phys. Rev. Lett. 119, 075502 (2017) [3] F. Perakis et al., Nat. Commun., 9, 1917 (2018).

Symposium : **ANAL1-3**

Advanced Instrumental Analysis Chemistry for Protein Dynamics Studies

Room 202, THU 16:30

Chair: Youngbok Lee (Hanyang University)

Correlative Super-Resolution Microscopy

Doory Kim

Department of Chemistry, Hanyang University, Korea

The rise of super-resolution microscopy (SRM, Research field of the Nobel Prize in Chemistry 2014, Technologies to watch in 2019 by Nature) over the past decade has drastically improved the resolution of light microscopy to ~ 10 nm, thus creating exciting new opportunities and challenges for correlative microscopy. Correlative microscopy, the integration of two or more microscopy techniques performed on the same sample, produces results that emphasize the strengths of each technique while offsetting their individual weaknesses. The new opportunities afforded by correlative SRM have hence motivated extensive new research, providing multidimensional, multi-scale, and corroborated information about a system regarding morphology, functionality, dynamics, cellular context, and chemical composition. In this presentation, I will talk about our technology development and recent applications of correlative SRM and other microscopy techniques, including electron microscopy, live-cell imaging, and spectroscopy. Using this approach, we studied filamentous influenza viruses, the purine biosynthetic enzymes organization complex called purinosomes, and the ring-opening reaction of photochromism molecules.

Symposium : **ANAL1-4**

Advanced Instrumental Analysis Chemistry for Protein Dynamics Studies

Room 202, THU 16:55

Chair: Youngbok Lee (Hanyang University)

Protein Design and Enzyme Evolution using X-ray Crystallography

Woon Ju Song

Department of Chemistry, Seoul National University, Korea

Nature utilizes numerous transition metal ions for dedicated chemical reactions. To explore the chemical reactivities of transition metal ions in proteinaceous environments, we have treated proteins as multi-functional ligands of which sequence can be easily altered by site-directed mutagenesis and directed evolution. Due to the structural flexibility and dynamic protein motions, we have applied X-ray crystallography to design the macromolecular ligands and to monitor the consequence of amino acid substitutions. We have designed Zn-dependent metallo-hydrolases from a structurally and functionally unrelated alpha-helical protein. From the comparative studies of two de novo metalloenzymes, we propose that at least three factors might be involved in the determination of catalytic activities and/or evolvability. In addition, we recently expand the targets from alpha-helical proteins to beta-barrel membrane proteins for protein engineering. Due to the intrinsic structural and chemical features of the protein platform, unprecedented metal-coordination and enzymatic activities have been observed with the de novo metalloenzymes. Our works suggest that proteins are versatile ligands of which function and structure can be modulated by the introduction of metal-ligand coordination bonds and that we can develop novel protein-based catalysts and materials.

Symposium : **ANAL2-1**

Analytical Technologies to Improve Human Health

Room 202, FRI 14:30

Chair: Hyun Joo An (Chungnam National University)

Reference Proteome-Based Subtyping of Liver Cancer

J. Eugene Lee

Center for Bioanalysis, Korea Research Institute of Standards and Science, Korea

Classification of hepatocellular carcinoma (HCC) into clinical subtypes is in high demand for the selection of proper treatment. For patients with HCC who are not or no longer candidates for locoregional therapy, oral multikinase inhibitors are the only established systemic alternative. Yet, the response rate of these FDA-approved drugs against HCC are less than one percent. Here, we adopted quantitative proteomic approaches in an attempt to characterize HCC subtypes in proteome level, and link these subtypes to drug response. We developed a liver reference proteome, a mixture of equal amounts of total proteins from seven liver cancer cell lines metabolically labeled with stable isotopes. This labeled reference proteome was utilized to cross-compare protein abundances from ten liver cancer cell lines that are widely used in research. Shotgun proteomic analysis on a hybrid quadrupole-orbitrap mass spectrometer with high mass accuracy at the MS and MS/MS levels yielded a liver proteome composed of 8,999 identified proteins, spanning 7 orders of magnitude in signal intensity. High-accuracy quantification allowed robust differentiation of HCC subtypes by principal component analysis. Furthermore, our liver reference proteome is being applied to quantify proteomes from liver cancer tissues collected from patients. HCC characterization by proteome expression may facilitate the establishment of clinical guidelines for subtype-specific systemic therapy.

Symposium : **ANAL2-2**

Analytical Technologies to Improve Human Health

Room 202, FRI 14:55

Chair: Hyun Joo An (Chungnam National University)

Electron microscopy study of nanomaterials

Young Heon Kim

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

The use of nanomaterials and related materials increases with the advance in the field of nanotechnology and the development of new industrial applications of nanoobjects. Although many scientific studies have been conducted for evaluating health and environmental risks of nanomaterials and related compounds, there are many controversial issues to be discussed. The starting point of the study on the toxicity and/or safety of nanomaterials is to precisely define the physicochemical properties. Electron microscopy (EM) techniques, based on scanning electron microscope and transmission electron microscope, have been found to be an indispensable tool for characterizing the physicochemical properties of nanomaterials due to its excellent spatial and energy resolutions. There have been many activities to establish standards for the measurement of nanoparticle size distribution by using various EM techniques. The morphology of nanomaterials can be also deduced through imaging and diffraction techniques in the EM. In addition, advanced in-situ TEM techniques enables us to explore unique and specific properties of individual nano-objects in the instrument. In this talk, I will show the research activities to develop traceable and reliable procedures for the measurement of particle size distribution by TEM. The results of inter-laboratory comparison studies for standardization, conducted in the various frameworks and/or programs, are introduced. Finally, the advanced TEM techniques to investigate the fascinating properties of nanomaterials is briefly demonstrated.

Symposium : **ANAL2-3**

Analytical Technologies to Improve Human Health

Room 202, FRI 15:20

Chair: Hyun Joo An (Chungnam National University)

Gastric Cancer Ascites Proteome for Potential Gastric Cancer Biomarkers Using Targeted Quantitative Methods

Jonghwa Jin

Division of Convergence Technology, New Drug Development Center, Korea

Gastric cancer is one of the most lethal malignancies, and the lack of specific early screening, diagnostic, and prognostic methods for such patients has necessitated the development of gastric cancer-specific biomarkers. Ascites is an important source of biomarkers, because it contains secreted proteins from malignant cells, growth factors, and cytokines. We performed a comprehensive proteome study using the ascites of patients with inflammatory diseases and gastric cancer. In the discovery stage, we identified 2761 ascites-specific proteins, 234 of which were quantitated by label-free quantitation using normalized spectral abundance factors (NSAFs)—152 and 82 proteins were up- and downregulated, respectively. In the verification stage (68 target proteins), we developed 2 quantitative targeted methods using stable isotope standard (SIS) peptide-based approaches—parallel reaction monitoring (PRM) and multiple reaction monitoring (MRM)—which target peptide fragments selectively and sensitively in complex samples; the PRM-targeted method showed high correlation with the MRM results (approximately 90% of peptides with $r > 0.9$). In the linear mixed effects analysis of the 2 methods, the expression of 36 proteins differed significantly between benign (N: 15) and cancer ascites (N: 33). Further, we performed a multiplex assay (linear discriminant analysis) using 7 biomarker candidates from the PRM and MRM analysis, resulting in a merged AUC value of 0.97 for PRM and 0.96 for MRM. Although our model requires further validation in a larger sample size, our 6- and 4-protein marker panel can be used as baseline references for the discovery of novel gastric cancer-specific biomarkers.

Symposium : **ANAL2-4**

Analytical Technologies to Improve Human Health

Room 202, FRI 15:45

Chair: Hyun Joo An (Chungnam National University)

Mass spectrometric approaches toward clinical proteomics

Jin Young Kim

Biomedical Omics Research Group, Korea Basic Science Institute, Korea

In proteomics aiming the biomarker discovery and development, mass spectrometer (MS) is an important analytical tool and is increasingly used for the investigation of clinical samples. Recent advances in protein or peptide separation and identification techniques have significantly improved proteomic approaches, leading to increase analytical performances such as specificity, sensitivity, throughput and robustness required for the successful clinical applications. In here, we will present the MS approaches and successes we have attempted to improve the analytical performance. There is mainly focused on MS based glycoproteomics including PRM-MS method combined with immunoprecipitation for the direct monitoring of glycopeptide targets in low abundant from serum and the high temperature LC-MS method for the enhanced separation of glycopeptide isomers.

Symposium : **ANAL2-5**

Analytical Technologies to Improve Human Health

Room 202, FRI 16:10

Chair: Hyun Joo An (Chungnam National University)

Using Mass Spectrometry to Probe for Potential Rheumatoid Arthritis Biomarkers

Youjin Seo

Analytical Research Center, Korean Institute of Toxicology, Korea

Rheumatoid arthritis (RA) is an autoimmune inflammatory disorder associated with redness, warmth, swelling and acute pain within joint linings. Current means of diagnosing RA involve blood test, x-rays and MRI. Any combinations of these tests, however, fail to live up to consistent accuracy when diagnosing RA, potentially resulting in inadequate or improper therapies administrated by health care professionals. In order to find better means of diagnosing RA, research showed that the release of glycosaminoglycans (GAGs), heterogeneous and linear polysaccharides consisting of disaccharide repeat units, occurred during inflammation and infection. In order to better understand the role GAGs have in RA, we used an LC-MS/MS platform to analyze GAGs derived from healthy and RA infected human sera. We established mass spectrometry methods to quantify GAGs and obtained specific information on their sulfation and/or acetylation patterning at a hexuronic acid and hexosamine. Our investigation discovered statistically significant difference in the sulfation and acetylation patterns between RA and healthy sera. Furthermore, since isomers of the disaccharide exist, we established a MS method that generated diagnostic ions capable of distinguishing the eight additional disaccharide isomers. This mass spectrometry method may further increase the overall accuracy of RA diagnoses.

Symposium : **LIFE1-1**

Recent Trends in Biopharmaceuticals Research

Room 303, THU 15:40

Chair: Jiwon Seo (GIST)

Core Competences in the Biopharmaceutical Development

Young-Phil Lee

Samsung Bioepis, Korea

The biopharmaceuticals account for 27% of the pharmaceutical market. Moreover, seven biopharmaceuticals are listed on the top 10 best-selling drugs. However, such seemingly promising market presents obstacles for market entry. Larger molecular weight of biopharmaceuticals in comparison to that of synthetic drugs makes biopharmaceuticals difficult to develop manufacturing processes and more vulnerable to quality changes by subtle process changes. Topping off the developmental hurdles, the pharmaceutical sector is one of the most regulated industries. Hence, in order to link science and knowledge gained from basic research to commercialization, it is necessary not only to overcome developmental hurdles, but also to obtain a marketing approval in compliance with the regulations of health authorities. Until now, most domestic pharmaceutical and bio-venture companies have repeatedly taken a cycle of licensing out candidate drugs to global pharmaceutical companies in the early stages due to lack of global development capabilities and experience and limited development costs. Under such circumstances, Samsung Bios and Celltrion have been striving to establish the commercialization capabilities of biopharmaceuticals in Korea, and achieved great success comparable to global standards in terms of the development, production and regulatory approval. Established in 2012, Samsung Bioepis is a biopharmaceutical company focused on increasing patient access to high-quality medicines through the development of biosimilars. Samsung Bioepis has launched 4 biosimilar products in Europe and in the U.S over the past 6 years. In this session, I will review the core competencies of Samsung Bioepis and present a vision to promote symbiosis for the globalization of the Korean pharmaceutical industry.

Symposium : **LIFE1-2**

Recent Trends in Biopharmaceuticals Research

Room 303, THU 16:10

Chair: Jiwon Seo (GIST)

Cellular cytosol-penetrating antibody technology and its applications

Yong-Sung Kim

Department of Applied Chemistry & Biological Engineering, Ajou University, Korea

Our group recently developed a platform technology of cellular cytosol-penetrating antibody (cytotransmab), which in the IgG format can reach the cytosolic space of living cells owing to its endosomal escaping ability after receptor-mediated endocytosis. Based on the cytotransmab technology, we have engineered human IgG1 format antibody, named iMab, which specifically internalizes into the cytosol of tumor cells and then selectively binds to targeted cytosolic proteins, including oncogenic Ras mutants. In this talk, I will present an innovative antibody technology that directly targets intracellular oncogenic KRas mutants to block the function from outside of cells after systemic administration. Our studies also demonstrate the feasibility of developing antibody therapeutics that directly target cytosolic proteins involved in disease-associated protein-protein interactions.

Symposium : **LIFE1-3**

Recent Trends in Biopharmaceuticals Research

Room 303, THU 16:40

Chair: Jiwon Seo (GIST)

Development of next-generation therapeutic antibodies through directed evolution

Sang Taek Jung

Department of Applied Chemistry, Kookmin University, Korea

IgG antibodies have been widely capitalized for therapeutics, diagnostics, and biomedical research reagents due to their outstanding target specificity and evolvability. For efficient isolation of monoclonal antibodies against highly valuable targets (e.g., soluble oncogenic targets, receptors, toxins, etc.) in a high throughput manner, we have constructed multiple human antibody libraries, which have a vast diversity of over 1×10^{11} , and have successfully utilized them for the isolation of monoclonal antibodies against highly challenging target antigens including G protein-coupled receptors. After binding to antigen, antibody Fc region determines therapeutic efficacy and serum half-life by the interaction with the Fc binding ligands such as Fc γ Rs (Fc gamma receptors), serum complement molecules, and FcRn (neonatal Fc receptor). To overcome the limitation of conventional monoclonal antibodies used in the clinical practice, engineering efforts in the last several years opened a new gateway to transform IgG Fc into a highly evolvable unit for a new desired function. To enhance therapeutic efficacy and circulating half-life, we have employed a variety of genetic, cellular and evolutionary strategies and the results will be discussed.

Symposium : **LIFE1-4**

Recent Trends in Biopharmaceuticals Research

Room 303, THU 17:10

Chair: Jiwon Seo (GIST)

Peptidomimetics Targeting Polo-Box Domain of Polo-like kinase 1

Jeong-kyu Bang

Korea Basic Science Institute, Korea

The serine/threonine kinase Polo-like kinase 1 (Plk1) is a regulator of multiple stages of mitotic progression. Several Plk1 kinase inhibitors have been uniformly demonstrated to induce mitotic arrest and apoptosis of cancer cells in vitro and in vivo. The PBD is unique to the family of PLKs and therefore it is ideally suited for studying the feasibility of inhibiting PLK1 by selectively influencing its protein-protein interaction. We have tried to develop the short peptidomimetic Plk1 PBD inhibitors with enhanced binding affinity and selectivity against Plk1 PBD from closely related Plk2 and Plk3. To achieve the desired short peptidomimetic agents, a systematic deletion and the N-terminal capping using diverse organic moieties were effected over the most potent 4j peptide, which led to the identification of AB-103 series with improved binding affinity and selectivity. In addition, AB-103 and their PEG-conjugated compounds were evaluated against their cellular uptake, anti-proliferation and Plk1 kinase inhibition by direct incubation with HeLa cells. Finally, improved binding affinity and selectivity of our derived compounds are explained by crystallographic evidences

Award Lecture in Division : **LIFE2-1**

Mass Spectrometry in Chemical Biology

Room 407+408, FRI 09:00

Chair: Jun-Seok Lee (KIST)

Investigation of Dynamic Features of Proteins Using NMR Spectroscopy

Yangmee Kim

Department of Bioscience and Biotechnology, Konkuk University, Korea

Flexibilities in protein conformations are essential for their functions. The relationship between protein structure, dynamics, and function is very challenging to study because the conformational space available to a protein is extensive and the time scales of conformational motions range widely, from picoseconds to seconds. These time scales are accessible by solution NMR making it a suitable technique for investigating the motions in proteins. Loop regions connecting secondary structural elements are highly dynamic and their motions play important roles in protein function. For example, the flexibility of the WPD loop as well as P-loop of phosphatase is closely related to its catalytic activity. Relaxation dispersion measurements can provide the closing rate of loops in phosphatases which play a role in the substrate recognition. The flexible recognition loops in acyl carrier protein (ACP) play key roles in communication with proteins in fatty acid synthase (FAS). We investigated these interactions between ACP and bacterial FAS proteins, which can be good targets for development of antibiotics. Also, the surface loop flexibility of cold shock protein is important to accommodate nucleic acids upon cold shock. The importance of dynamic features of proteins for their molecular recognition processes and their catalytic activities will be demonstrated using spin relaxation approaches, showing that solution NMR spectroscopy is a strong tool for study of protein dynamics and functional consequences.

Symposium : **LIFE2-2**

Mass Spectrometry in Chemical Biology

Room 407+408, FRI 09:30

Chair: Jun-Seok Lee (KIST)

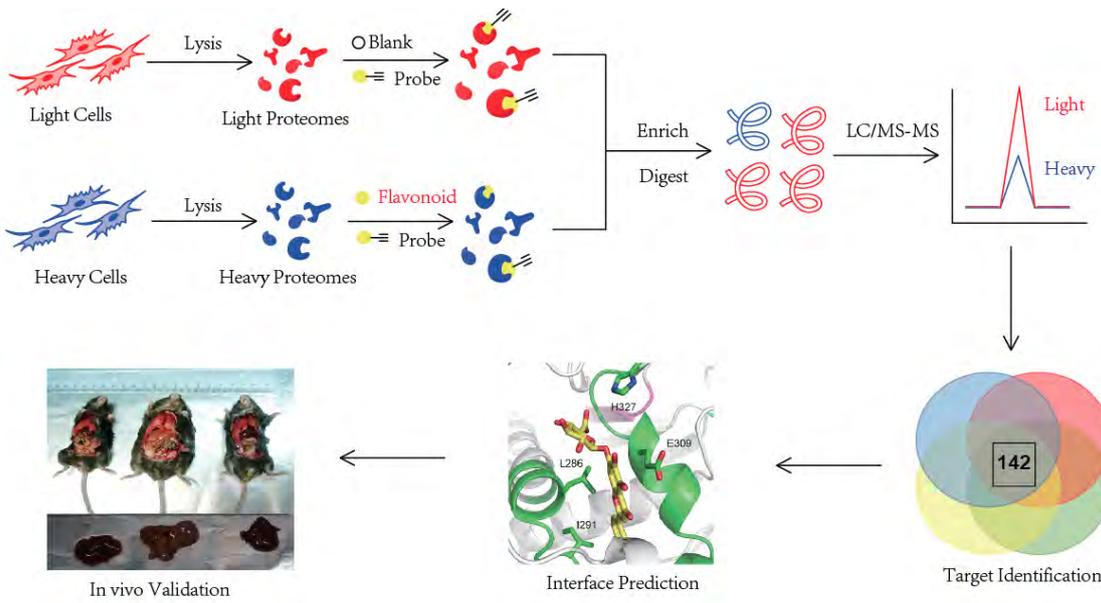
Chemical and Computational Proteomics for Functional Target Discovery

Chu WANG

College of Chemistry and Molecular Engineering, Peking University, Beijing, China

Genome sequencing projects have revolutionized our view of the complexity of prokaryotic and eukaryotic proteomes, however, we are also left with a daunting challenge of functionally annotating these large number of predicted proteins. Chemical proteomic methods, such as activity-based protein profiling (ABPP), have been developed aiming at systematically discovering new functional targets directly from native proteomes. In this talk, I will present a recent project from my laboratory which combine ABPP-based chemical proteomic, biochemical and computational strategies to uncover the functional targets of a specific bioactive ligand in proteomes.

Hepatic steatosis, marked as excessive lipid accumulation in hepatocytes, constitutes the early stage of non-alcoholic fatty liver diseases (NAFLD) which could eventually lead to liver cancer. The pathogenic mechanism for this lipid metabolism imbalance remains elusive and an effective treatment option is yet to be developed. In the current work¹, we showed that a flavonoid compound isolated from the Chinese traditional herbal medicine is an effective anti-steatosis agent. By employing a quantitative activity-based protein profiling (ABPP) strategy, we discovered the flavonoid binds to key enzymes in the fatty acid metabolic pathway, accelerate the metabolic rate of fatty acids in the liver and ameliorates the symptoms associated with hepatic steatosis. We performed computational docking studies to map the potential protein-ligand interface and mutation of the predicted interface residues completely abolished the bioactivity of the flavonoid compound, confirming that it acts mechanistically through the enzyme to confer the anti-steatosis effect. Based on the finding, we also screened multiple representative flavonoid compounds and found new potential lead compounds to further enhance the activation effect on the enzyme. Our data indicate that regulating the fatty acid metabolism is an effective approach to prevent hepatic steatosis and the flavonoid may serve as a common scaffold to develop novel drugs for pharmacological treatment of NAFLD.



Symposium : **LIFE2-3**

Mass Spectrometry in Chemical Biology

Room 407+408, FRI 10:00

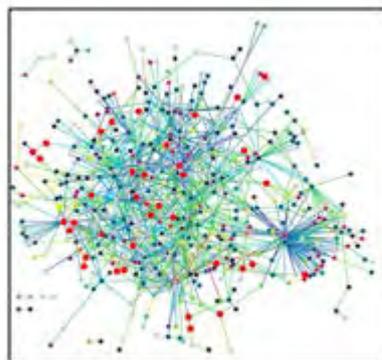
Chair: Jun-Seok Lee (KIST)

In vivo proteome mapping by proximity labeling

Hyun-Woo Rhee

Department of Chemistry, Seoul National University, Korea

Recently, proximity labelling methods have been developed to map spatially localized proteome in live cells. Usually, these methods employ enzymatic biotinylation of the proximal proteins with short-lived reactive biotin species. The labeled proteins may contain biotinylated modifications, which can be detected by mass spectrometry after enrichment by streptavidin bead affinity purification. Using the direct detection method of biotinylated proteins by mass spec (Spot-ID), we could reveal the in vivo topological direction of 135 inner-mitochondrial membrane (IMM) proteins by an in situ-generated radical probe with genetically targeted peroxidase (APEX) in live cells. Furthermore, we could identify the global topological information of the porous outer mitochondrial membrane proteome in live cells by using isotope-coded probes. From these results, we could see that our methods may have a great potential to reveal other sub-compartmental membrane proteomic architecture in live cells. Currently, we further extend this method to reveal in vivo mitochondrial proteome of different tissues and organs of the animal model.



Symposium : **LIFE2-4**

Mass Spectrometry in Chemical Biology

Room 407+408, FRI 10:20

Chair: Jun-Seok Lee (KIST)

Secondary Structural Study of Biomolecules and Their Assemblies Using IM-MS and Gas-Phase IR Spectroscopy

Jongcheol Seo

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

Mass spectrometry has been a routine tool for identifying and analyzing various biological molecules. Most recently, the structural studies of peptides, proteins, and their assemblies using MS-based methods firstly came to light in the developments of native mass spectrometry using very soft nano-electrospray ionization and have been significantly extended by emerging ion mobility mass spectrometry. However, the key question in this field has been whether the structures of biomolecules and their assemblies can be actually determined by using mass spectrometry-based gas-phase methods. Furthermore, it is also not clear if the structural elements of biomolecules are conserved after transfer to the gas phase via ionization. A clarification of this problem is important since it would allow very sensitive native mass spectrometry to be used to address problems relevant to structural biology. We used a combination of ion mobility-mass spectrometry (IM-MS) and gas-phase infrared spectroscopy to investigate the structures of biomolecules from small metabolite to peptides and proteins. Firstly, the secondary and tertiary structure of proteins transferred from solution to the gas phase was investigated. The results show that for low charge states under gentle ionization conditions, aspects of the native secondary and tertiary structure can be conserved. Based on this result, we further investigated amyloidogenic peptide aggregates and succeeded the first direct secondary structural analysis of every individual amyloid intermediate from dimer up to dodecamer. These results clearly suggest that the ion mobility-mass spectrometry can be used to investigate the secondary structures of proteins, peptides, and their aggregates.

Symposium : **LIFE2-5**

Mass Spectrometry in Chemical Biology

Room 407+408, FRI 10:40

Chair: Jun-Seok Lee (KIST)

Multiplexed proteome quantification platform using isotopic chemical and metabolic labeling

Jong-Seo Kim

Center for RNA Research, IBS, Seoul National University, Korea

Isotopic labeling allows for highly accurate and reliable quantification in mass spectrometry-based proteomics. The major technical hurdle, however, is the limited multiplexity (e.g., triplex in SILAC) owing to issues regarding the signal overlapping of isotopic peptide forms and the chromatographic retention time shift. Herein, we present a novel multiplexed MS1-level quantification platform that comprises new six-plex in vivo SILAC or in vitro di-ethylation with a dedicated algorithm, EPIQ (Epic Protein Integrative Quantification). We show that EPIQ significantly outperforms the current state-of-the-art tools and allows for highly specific and sensitive detection of differentially expressed proteins without the need for high-end instrumentation. EPIQ together with highly-multiplexed isotopic labeling schemes may offer new opportunities for studies on protein dynamics via metabolic labeling and for clinical proteomic analyses relying on accurate protein quantification.

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

Current Trends in Organic Chemistry I : Synthetic Methodology and Application

Room 301+302, THU 15:40

Chair: Wonsuk Kim (Ewha Womans University)

Development of New Catalytic Transformations: Efficient and Selective Construction of Various N-Heterocycles

So Won Youn

Center for New Directions in Organic Synthesis, Department of Chemistry, Hanyang University, Korea

Our research group has been interested in the development of new and efficient catalytic synthetic methods. Especially, we have been making efforts to develop effective one-pot protocols by using metal catalysts for heterocyclic synthesis. Since complicated molecules can be directly constructed from readily available starting materials under relatively mild conditions in an unprecedented manner, the direct and selective C-H bond functionalization plays a crucial role in preparing a wide range of biologically and physically important organic molecules, providing significant advantages over traditional synthetic methods. Moreover, one-pot reactions that involve a sequence of chemical transformations in a single flask are much desired as a powerful tool for the construction of various complex molecules from simple starting materials. In this presentation, our recent discovery of several efficient Pd-catalyzed transformations will be described. These synthetic methods provided mild, simple, and efficient routes with high regio- and/or stereoselectivities to valuable N-heterocycles such as indoles, carbazoles, and isoindolinones which are important motifs in bioactive natural products, pharmaceuticals, and other functional molecules.

Symposium : **ORGN1-2**

Current Trends in Organic Chemistry I : Synthetic Methodology and Application

Room 301+302, THU 16:10

Chair: Wonsuk Kim (Ewha Womans University)

Synthetic Strategies for the Conjugated Polyene Chains of Carotenoids

Sangho Koo

Department of Chemistry, Myongji University, Korea

Carotenoids are structurally interesting natural products containing the conjugated polyene chains of nine carbon-carbon double bonds, which exhibit antioxidant activity by scavenging reactive oxygen species (ROS). Certain carotenoids have vitamin A activity for cell growth and differentiation, and thus widely used as nutrition and drug. They are also utilized as coloring agents for foods and cosmetics due to their distinctive red colors. Various synthetic strategies for the conjugated polyene chains of the carotenoids will be discussed with special emphasis on the utilization of functionalized C5 and C10 units, designed for efficient construction of the carotenoids with nonpolar or polar terminal groups. C20 building blocks were devised for expeditious assembly of carotenoids, which allowed SAR of the terminal structures on the antioxidant activity of carotenoids by high throughput screening and hierarchical clustering analysis of ABTS and DPPH radical scavenging assays.

Symposium : **ORGN1-3**

Current Trends in Organic Chemistry I : Synthetic Methodology and Application

Room 301+302, THU 16:35

Chair: Wonsuk Kim (Ewha Womans University)

α -Vinyl Enolization of β -Chlorovinyl Ketones: Pathway Discovery and Synthetic Utility

Hun young Kim

College of Pharmacy, Chung-Ang University, Korea

In contrast to other α , β -unsaturated carbonyl compounds, a mild base-promoted α -vinyl enolization of β -chlorovinyl ketones allows the generation of unique intermediate species with nucleophilic or electrophilic reactivity. We have disclosed the synthetic utilities of β -chlorovinyl ketones based on a α -vinyl enolization strategy. However, one drawback in this strategy, especially in terms of reaction efficacy, is that the planar conformation of (Z)- β -chlorovinyl ketones displays a α -vinyl enolization significantly slower than that of (E)- β -chlorovinyl ketones. The tedious separation of (E)- β -chlorovinyl ketones from (Z)- β -chlorovinyl ketones and the lack of efficient synthetic methods to (E)- β -chlorovinyl ketones became the bottleneck in the synthetic utilization of β -chlorovinyl ketones via α -vinyl enolization. To improve efficacy of this strategy, we have explored two approaches: 1) microwave-assisted thermal α -vinyl enolization of β -chlorovinyl ketones, 2) (E)-selective Friedel-Crafts acylation of alkynes to β -chlorovinyl ketones by flow chemistry. In this talk, we will present an efficient synthetic transformation of stereoisomeric β -chlorovinyl ketones using ring-expansion, ring-opening, and cycloisomerization strategies with the discovery of a microwave-assisted thermal α -vinyl enolization of β -chlorovinyl ketones. The mixtures of (E/Z)- β -chlorovinyl ketones are directly employed without separation in this thermal α -vinyl enolization approach. Also, a flow chemistry approach will be introduced as a fast, high yielding, and stereoselective synthetic route to (E)- β -chlorovinyl ketones. The (E)/(Z) isomerization under the $AlCl_3$ -promoted Friedel-Crafts reaction conditions is prevented via the product segregation strategy using a flow chemistry system.

Symposium : **ORGN1-4**

Current Trends in Organic Chemistry I : Synthetic Methodology and Application

Room 301+302, THU 17:10

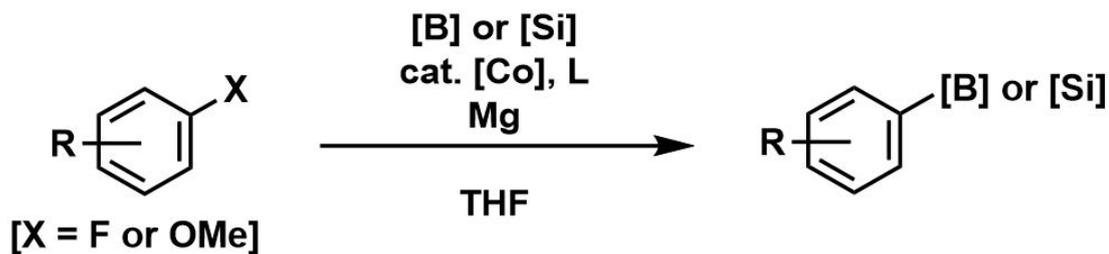
Chair: Wonsuk Kim (Ewha Womans University)

Cobalt-catalyzed Functionalization of Inert Aryl-X Bonds

Eunsung Lee

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

Functionalization of inert bonds in arenes such as C_{aryl}-F and C_{aryl}-OMe has been a promising synthetic tool for accessing a variety of new organic substrates because C_{aryl}-F and C_{aryl}-OMe bonds are very stable so that they can be survived for last-stage functionalization of those bonds. Therefore, significant efforts have been put for selective functionalization of C_{aryl}-F and C_{aryl}-OMe bonds for the past decades. Our group has been developing cobalt catalysis that enables such a transformation. Recently, we reported the first cobalt-catalyzed borylation of C_{aryl}-F bond.¹ Associated with the project, we successfully incorporate the methodology to functionalize C_{aryl}-F and C_{aryl}-OMe bonds with boryl and silyl groups. The details will be discussed. 1.Lim, S.; Song, D.; Jeon, S.; Kim, H.; Lee, S.; Cho, H.; Lee, B. C.; Kim, S. E.; Kim, K.; Lee, E. *Org. Lett.* 2018, 20, 7249.



Symposium : **ORGN1-5**

Current Trends in Organic Chemistry I : Synthetic Methodology and Application

Room 301+302, THU 17:35

Chair: Wonsuk Kim (Ewha Womans University)

Copper-Catalyzed Tandem C–B and C–C Bond Formation for Asymmetric Synthesis of Organoboron Compounds

Jaesook Yun

Department of Chemistry, Sungkyunkwan University, Korea

Development of efficient synthetic methods of organoboron compounds has attracted significant attention over the years due to their versatility in organic synthesis. We previously reported that a copper(I)-boryl complex coordinated with chelating bisphosphines reacted with vinyl arenes regio- and enantioselectively to form a chiral benzyl organocopper intermediate. The organocopper species was subsequently consumed in a tandem catalytic cycle for further C–C bond formation such as allylation. In this seminar, I will present our recent progress in asymmetric tandem reactions using organocopper species generated by in-situ borylcupration.

Symposium : **ORGN2-1**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 301+302, FRI 09:00

Chair: In Su Kim (Sungkyunkwan University)

Synthesis of Indole Derivatives Using Diazoindolinimines

Phil Ho Lee

Department of Chemistry, Kangwon National University, Korea

Rh-catalyzed cyclization reaction of sulfoximines with 3-diazoindolinimines is described. This protocol provided a wide range of indolobenzothiazines together with the release of molecular nitrogen and *p*-toluenesulfonamide. The present method involved the N-H/C-H activation of *S*-aryl sulfoximines and has the advantages of a broad substrate scope. A regioselective synthetic method for the preparation of pyrazinoindoles was demonstrated 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 pyrazinoindoles, the present method using unsymmetrical azirines has a strong advantage from a regioselectivity viewpoint. Rh-catalyzed formal aza-[4 + 3] cycloaddition reaction of 3-diazoindolinimines with 1,3-dienes was demonstrated for the synthesis of azepinoindoles in one-pot. First, Rh-catalyzed [2 + 1] cycloaddition reaction smoothly took place to produce iminyl vinyl cyclopropane intermediate at room temperature in chlorobenzene, which was thermally converted to azepinoindoles via aza-Cope rearrangement.

Symposium : **ORGN2-2**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 301+302, FRI 09:25

Chair: In Su Kim (Sungkyunkwan University)

Iron-polypyridyl Complexes in Single Electron Transfer Strategy for Cycloaddition Reactions

Eun Joo Kang

Department of Applied Chemistry, Kyung Hee University, Korea

Transition metal complexes with polypyridyl ligands have been used as important catalysts in single-electron-transfer (SET) organic reactions. Especially, photoredox organic reactions such as radical coupling reactions and oxidative/reductive cyclization reactions were developed by using Ru, Ir, Ni, and Cu polypyridyl complexes as photocatalysts. Iron polypyridyl complexes is not a good candidate for photoinduced electron transfer catalysis due to the short lifetime of the lowest energy excited state. However, Cozzi and Ceroni reported [Fe(bpy)₃]Br₂ catalyzed organocatalytic enantioselective alkylation of aldehydes in 2015, and Collins's group reported [Fe(phen)₃](NTf₂)₂ catalyzed photochemical synthesis of carbazole under continuous flow conditions. Iron(III) polypyridyl complexes exhibit the proper potential as single-electron oxidants with tertiary amines or anilines [E_{ox} = 0.8-1.0 V] for formation amine radical cation. After amine is oxidized by iron(III) complex, deprotonation of amine radical cation offers α-amino radical species, which is reactive to α,β-unsaturated carbonyl compounds as a radical acceptors. Herein, the oxidative cycloaddition of tertiary amines with maleimides under mild reaction condition will be presented. Additionally, iron(III) polypyridyl complexes have sufficient potential as single-electron oxidant to oxidize electron-rich styrenes, thereby promoting efficient radical cation cycloaddition with electron-rich dienophiles. The novel and innovative approach using Fe(III) complexes as effective radical generator can be a facile route to replace rare metals with inexpensive and sustainable iron complexes, one of the five most abundant metals in the Earth's crust.

Symposium : **ORGN2-3**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 301+302, FRI 10:00

Chair: In Su Kim (Sungkyunkwan University)

Pd-catalyzed polymerization using carbon monoxide

Hye-Young Jang

Department of Energy Systems Research, Ajou University, Korea

Carbon monoxide (CO) is considered a useful C1 source; the utilization of CO in the chemical conversion has been studied for a long time, developing various commercial processes. In the field of polymer industries, polyketones are well-known polymers utilizing CO and ethylene/propylene. In addition to economic and environmental benefits of CO, polyketone shows attractive properties of engineering plastics which may replace current polymers. With these reasons, polyketone production was already commercialized in the mid of 1980s. However, there are a couple of critical issues of polyketone synthesis. One of the issues is polymer fouling stemming from the uncontrolled polymer growth. In this presentation, we will show how to control the polymer fouling by modifying palladium catalysts. References 1) Y. N. Lim, H.-W. Noh, Y.-J. Cheong, S. Y. Kang, B. Y. Lee, S. U. Son, H.-Y. Jang, ACS Sustainable Chem. & Eng. 2017, 5, 9657-9661. 2) Y. N. Lim, S. K. Chae, W. Yim, J.-Y. Park, W. Yoon, H. Yun, E. Kim, S. U. Son, H.-Y. Jang, Appl. Organomet. Chem. 2019, Early view

Symposium : **ORGN2-4**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 301+302, FRI 10:25

Chair: In Su Kim (Sungkyunkwan University)

Asymmetric Catalytic Cascade Reactions for the Synthesis of Chiral Fused-ring Compounds

Sung-Gon Kim

Department of Chemistry, Kyonggi University, Korea

Fused-ring structural units including chroman, indoline, pyrrolidine and hydroquinoline are widely distributed in nature and many biologically active compounds. Molecules containing these structural units exhibit a broad range of bioactivities such as anticancer, antiviral, antitumor, antimicrobial, sex pheromone, and central nervous system activity. Owing to the importance of these class of compounds, the stereoselective and enantioselective synthesis of fused-ring compounds is a noteworthy synthetic goal. In this presentation, I will demonstrate the asymmetric synthesis of hydroquinoline, hydroquinazoline, and hydroisoquinoline via catalytic cascade reaction in which mainly organocatalysts are used. As an example, the asymmetric reaction of 2-(tosylamino)phenyl α,β -unsaturated ketones with alkynyl aldehydes, promoted by diphenylprolinol *O*-TMS ether as an organocatalyst, generates chiral 1,4-dihydroquinolines in good to high yields with excellent enantioselectivities (up to 97% ee).

Symposium : **ORGN3-1**

Current Trends in Organic Chemistry III: Functional Organic Molecules

Room 301+302, FRI 14:30

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

Electric-Field Responsive Columnar Assemblies of 1,2,3-Triazole-based Liquid Crystals

Byoung-Ki Cho

Department of Chemistry, Dankook University, Korea

One dimensional (1D) columnar organization of π -conjugated aromatic building blocks is an interesting research topic because the electric and photophysical functions can be engineered by the orientation and packing order of columnar domains. Recently, we have studied columnar liquid crystals based on 1,2,3-triazole group which is capable of the hydrogen-bonding interaction and response to electric-field. As examples, we designed several columnar-forming molecules based on polar 1,2,3-triazole group. The columnar LC thin- and bulk-level films could be macroscopically aligned under E-field. The uniform orientation over a large film area could be achieved by a quick and easy E-field method. Moreover, an LC molecule consisting of a naphthalene core dominantly adopted cisoid conformer with non-zero dipole moment which organized into a double helical columnar structure in the LC state. The columnar LC structure showed a ferroelectrically switching property which is, to our knowledge, the first example containing triazole unit as the polar unit to date. The details regarding these issues will be addressed in the presentation.

Symposium : **ORGN3-2**

Current Trends in Organic Chemistry III: Functional Organic Molecules

Room 301+302, FRI 14:55

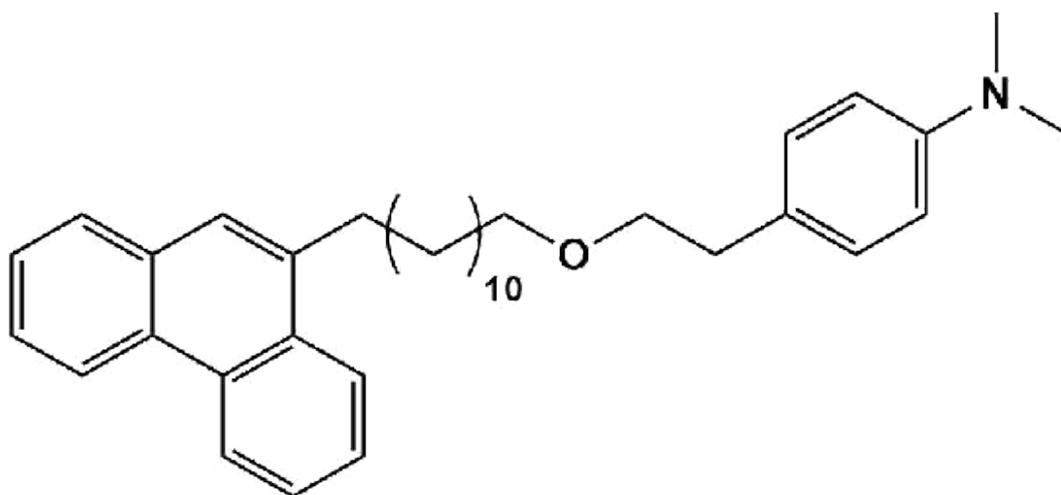
Chair: Min Hee Lee (Sookmyung Women's University)

Exciplex-based Magnetic Field-Sensitive Fluorophores

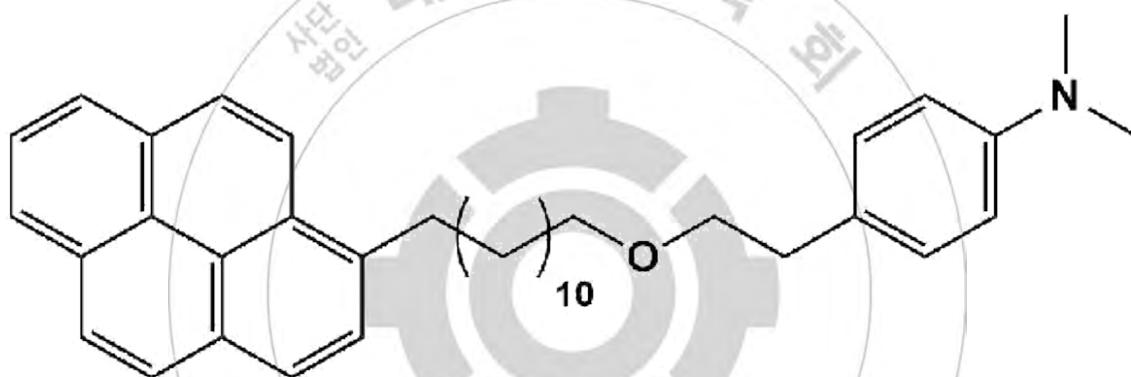
Hohjai Lee

Chemistry, Gwangju Institute of Science and Technology, Korea

Some chemical reactions are sensitive to external magnetic field. Majority of them are based on the radical-pair mechanism. Especially, when the radical pair system is in equilibrium with emissive exciplex, the amount of the emission can be modulated with the external magnetic field. In this talk, I will discuss magnetic field-sensitive fluorophores that are composed of chain-linked polyaromatic electron acceptor and amine electron donor, for an example, pyrene-(CH₂)₁₂-O-(CH₂)₂-*N,N*-dimethylaniline. I will demonstrate several fluorescence imaging techniques that were obtained with the fluorophores and introduce a fluorophore for practical applications of mapping the magnetic field. Under a 375-nm illumination, an image of magnetic field distribution is obtained with it. Its feasibility for obtaining a magnetic field image with two-photon fluorescence microscopy is demonstrated.



Phen-12-O-2-DMA (1)



Py-12-O-2-DMA (2)

Symposium : **ORGN3-3**

Current Trends in Organic Chemistry III: Functional Organic Molecules

Room 301+302, FRI 15:20

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

Organic Molecules For Cellular Uptake

Eun-Kyoung Bang

Center for Neuromedicine, Korea Institute of Science and Technology, Korea

In this talk, we briefly discuss about poly(disulfide)s and amphiphiles for use as novel siRNA transporters. First, dynamic polymers with disulfide repeats in their main chain, were developed to deliver biomolecules through the cellular membrane. We report the synthesis of the counterion propagator units and subsequent polymerization by ring-opening disulfide exchange.[1] We also show that the most active fluorescent poly(disulfide)s reach the cytosol of HeLa cells within 5 min and depolymerize in less than 1 min to release the native substrate. [2] As the second part, we report coordinative amphiphile as a siRNA transporters.[3] As a modification of a conventional cationic lipid structure, we replaced the cationic head with zinc(II)-dipicolylamine complex (Zn/DPA) as a phosphate-directing group, and used various membrane-directing groups in the place of the hydrophobic tails. Interestingly, the Zn/DPA head itself exhibited moderate transfection efficiency, and its combination with various membrane-directing groups enhanced the delivery efficiency without imparting significant cytotoxicity. Thus, it appears possible to develop tunable siRNA transporters simply by changing the membrane-directing parts. These are the first examples of amphiphilic siRNA transporters accompanying coordinative interactions between the amphiphiles and siRNAs. References [1] Bang, E.-K.; Gasparini, G.; Molinard, G.; Roux, A.; Sakai, N.; Matile S. J. Am. Chem. Soc. 2013, 135, 2088–2091. [2] Gasparini, G.; Bang, E.-K.; Molinard, G.; Tulumello, D. V.; Ward, S.; Kelley, S. O.; Roux, A.; Sakai, N.; Matile S. J. Am. Chem. Soc. 2014, 136, 6069–6074. [3] Kim, J. B.; Lee, Y. M.; Ryu, J.; Lee, E.; Kim, W. J.; Keum, G.; Bang, E.-K., Bioconjugate Chem. 2016, 27, 1850–1856.

Symposium : **MEDI-1**

The Cutting Edge of Drug Discovery Chemistry

Room 304, THU 15:40

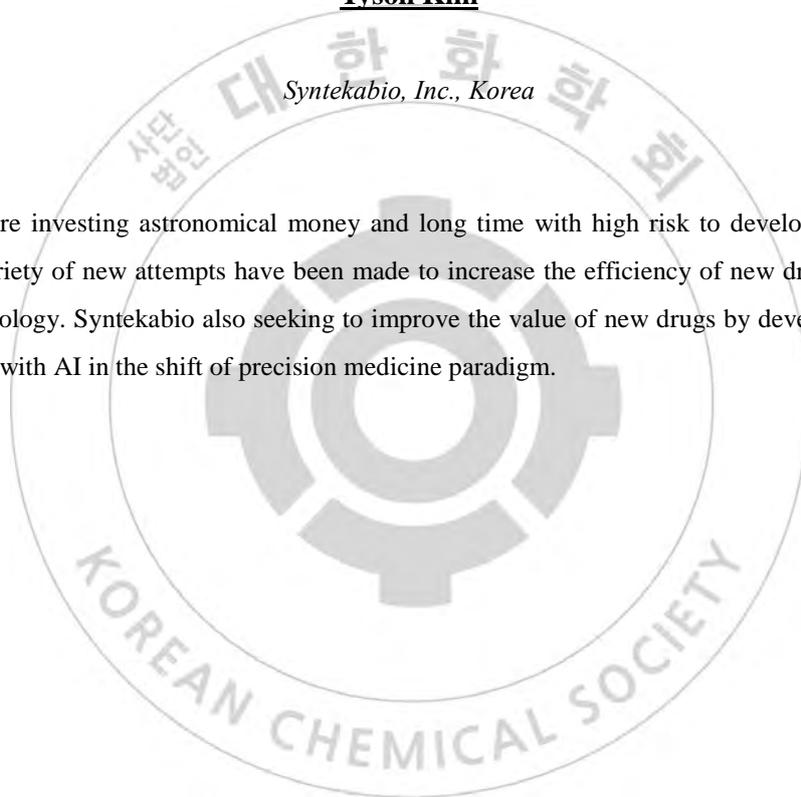
Chair: Sun-Joon Min (Hanyang University (ERICA))

AI Drug Discovery & Precision Medicine

Tyson Kim

Syntekabio, Inc., Korea

Big pharmas are investing astronomical money and long time with high risk to develop a blockbuster. Recently, a variety of new attempts have been made to increase the efficiency of new drug development using AI technology. Syntekabio also seeking to improve the value of new drugs by developing genome-based big data with AI in the shift of precision medicine paradigm.



Symposium : **MEDI-2**

The Cutting Edge of Drug Discovery Chemistry

Room 304, THU 16:10

Chair: Sun-Joon Min (Hanyang University (ERICA))

Development of NOV1701, direct c-Myc-DNA inhibitor, for novel anti-cancer treatment

Hwan Jung Lim

Information-Based Drug Research Center, Korea Research Institute of Chemical Technology, Korea

c-Myc has been known as one of the most potent oncoproteins. According to the report in 2005, more than 1/7 cancer deaths in US were related to deregulated c-Myc. Moreover, there are large numbers of studies which showed that c-Myc amplification induced diverse cancers, such as gastric cancer, colon cancer, small cell lung cancer, breast cancer, and leukemia. Although these clear evidences that c-Myc could be an effective target to develop a new anti-cancer drug, direct and selective regulation of c-Myc by a small-molecule is believed to be almost impossible. A few of direct c-Myc inhibitors such as F4 were reported, but none of them is enough to be a preclinical candidate. Other molecular targets such as BRD4 and SUMO activating enzyme 1/2 (SAE1/2) that can indirectly regulate c-Myc transcription has been actively pursued by many groups. In this presentation, brief developmental history of our small-molecular direct inhibitor NOV1701 will be shown. NOV1701 showed exceptional potencies toward our in-vitro and in-vivo assay systems. To other transcription factors such as AP-1 and Max-Max homodimer, it showed very high selectivities. ADME-T studies showed that NOV1701 have proper drug-like properties with low toxicities. In xenograft studies, PO administrated NOV1701 showed exceptional anti-tumor effects without body weight loss.

Symposium : **MEDI-3**

The Cutting Edge of Drug Discovery Chemistry

Room 304, THU 16:50

Chair: Jaeho Yoo (CJ HealthCare, New Drug Research Center)

Newly developed reversible MAO-B inhibitor circumvents the shortcomings of irreversible inhibitors in Alzheimer's disease

Ki Duk Park

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

Monoamine oxidase-B (MAO-B) has recently emerged as a potential therapeutic target for Alzheimer's disease (AD) due to its association with aberrant gamma aminobutyric acid (GABA) production in reactive astrocytes. Although short-term treatment with irreversible MAO-B inhibitors, such as selegiline, improves cognitive deficits in AD patients, long-term treatments have shown disappointing results. Here, we show that prolonged treatment with selegiline fails to reduce aberrant astrocytic GABA levels and rescue memory impairment in APP^{swe}/PSEN1^{dE9} (APP/PS1) mice, an animal model of AD, because of increased activity in compensatory genes for a GABA-synthesizing enzyme, diamine oxidase (DAO). We have developed a potent, highly selective, and reversible MAO-B inhibitor, KDS2010 (IC₅₀: 7.6 nM; 12,500-fold selectivity over MAO-A), which overcomes the disadvantages of the irreversible MAO-B inhibitor. Long-term treatment with KDS2010 does not induce the compensatory mechanisms, thereby significantly attenuating increased astrocytic GABA levels and astrogliosis, enhancing synaptic transmission, and rescuing learning and memory impairments in APP/PS1 mice.

Symposium : **MEDI-4**

The Cutting Edge of Drug Discovery Chemistry

Room 304, THU 17:20

Chair: Jaeho Yoo (CJ HealthCare, New Drug Research Center)

Discovery of Novel Pyruvate Dehydrogenase Kinase 4 Inhibitors for Potential Oral Treatment of Metabolic Diseases

Jin hee Ahn

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

Glycolysis, the initial stage of glucose metabolism, yields a two ATPs, two NADHs and two molecules of three-carbon compound pyruvate from glucose. Subsequently, pyruvate generated from glycolysis is catalyzed into acetyl-coenzyme A (Acetyl CoA) by pyruvate dehydrogenase complex (PDC). Acetyl CoA enters the tricarboxylic acid cycle and finally produces ATP, which is an energy source for the body. This cascade is coupled to the synthesis of 36 molecules of ATP by oxidative phosphorylation. The enzymatic activity of PDC is inhibited by pyruvate dehydrogenase kinases (PDK1-4) by phosphorylating three serine residues on its E1 α subunit ; Ser232, Ser293 and Ser300 with different specificity for each sites. Many previous studies have demonstrated that dysregulation of the PDH/PDK system is implicated in the onset of various diseases such as cancer, metabolic diseases, and inflammation, suggesting that PDKs are a potent therapeutic target for these diseases. Pyruvate dehydrogenase kinase 4 (PDK4) activation is associated with metabolic diseases including hyperglycemia, insulin resistance, allergies and cancer. GM compound showed promising in vitro activity with an IC₅₀ value of 84 nM. Good metabolic stability, pharmacokinetic profiles and possible metabolites were suggested. GM compound improved glucose tolerance in diet-induced obese mice and ameliorated allergic reactions in passive cutaneous anaphylaxis (PCA) mouse model. Additionally, GM compound exhibited anti-cancer activity by controlling cell proliferation, transformation, and apoptosis. From the molecular docking studies, GM compound displayed optimal fitting in the lipoamide binding site (allosteric) with a full fitness, providing a new scaffold for drug development towards PDK 4 inhibitors.

Symposium : **MAT1-1**

Synthesis and Application of Multifunctional Nanocatalyst Materials

Room 405+406, THU 15:40

Chair: Sang-II Choi (Kyungpook National University)

Toward ideal heterogeneous nanocatalysts

Kwangyeol Lee

Department of Chemistry, Korea University, Korea

Nanoparticle-based heterogeneous catalysis is intrinsically surface-confined, and thus it is advantageous to increase the surface area per mass of the nanocatalysts. The surface energy is also directly related to the activity of the nanocatalysts because the binding and detachment of the substrate, intermediates, and the final products require the optimal positioning of the nanoparticle surface energy. In order to enhance the activity, therefore, the design concepts of nanocatalysts have evolved to encompass the core-shell nanoparticles with lattice mismatch between core and shell, which would dramatically increase the surface energy, well-defined polyhedral nanocrystals with high index crystal facets, alloy nanoparticles with optimal d-band position, and eventually alloy nanoframes. There are pros and cons of these nanoparticles because, in general, very high activity of nanocatalysts is not compatible with the stability of them during catalysis. For example, nanoframes have been developed to maximally profit from the large surface area. However, their catalytic performances might rapidly deteriorate due to the collapse of the nanoframe structure consisting of tenuous connected nanowires. Therefore, we have a daunting task of developing nanocatalyst systems exhibiting all the desired properties of 1) high surface area, 2) high structural robustness, and 3) fine-tuned surface energy. In this seminar, I will describe our current efforts on development of ideally performing nanocatalysts for electrolytic water splitting and hydrogen fuel cells, which have received a great attention due to ever increasing environmental problems associated with fossil fuel usages. Specifically I will focus on the synthesis of multiphasic nanoparticles, which exhibit region-specifically located multiple material phases within a very small nanoparticle domain and eventually evolve into nanoframe catalysts with high surface area, high structural robustness, and fine-tuned surface energy. The nanoscale alloying process and atom exchange process, which is of a paramount importance to the formation of nanoframes with desired structural features, will be described in detail.

Symposium : **MAT1-2**

Synthesis and Application of Multifunctional Nanocatalyst Materials

Room 405+406, THU 16:05

Chair: Sang-II Choi (Kyungpook National University)

Advanced TiO₂ Nanomaterials for Photocatalytic Applications

Jongmin Choi

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

Titanium dioxide (TiO₂) is one of the most popular photocatalytic materials because of their abundance, low material cost, and outstanding chemical and photochemical stability. With these benefits, TiO₂ nanomaterials are widely applied in photocatalytic applications including hydrogen production, air pollutant degradation, water purifications etc. Despite their promising characteristics, several characteristics of TiO₂ stand to be improved further. For example, TiO₂ has narrow light harvesting absorption window, and TiO₂ nanoparticles, which is the most widely used TiO₂ nanostructure, suffers from the catalyst deactivation which is induced by the accumulation and strong adsorption of by-products induced by photocatalytic reactions. To address these issues, we developed freestanding doubly open-ended TiO₂ nanotube membrane via facile fabrication process and chemical engineering. These advanced TiO₂ nanomaterials demonstrated promising photocatalytic activities for water splitting and degradation of volatile organic compounds compared to those of conventional TiO₂ nanoparticles. In this presentation, I will introduce design, synthesis, engineering and applications of these advanced TiO₂ nanomaterials.

Symposium : **MAT1-3**

Synthesis and Application of Multifunctional Nanocatalyst Materials

Room 405+406, THU 16:30

Chair: Sang-II Choi (Kyungpook National University)

Earth-abundant Catalysts for Electrochemical and Photoelectrochemical Water Splitting

Ki Min Nam

Department of Chemistry, Pusan National University, Korea

Solar-driven water splitting to produce hydrogen and oxygen is a promising approach to convert sunlight into chemical fuels. Complete water splitting involves multi-electron and multi-proton transfer and is challenging from both thermodynamic and kinetic points of view. While many materials have been investigated for potential use in solar water splitting, one of the most critical issue is the development of efficient electrocatalysts for rapid surface kinetics on semiconductor photoelectrodes. The oxygen evolution reaction (OER) is particularly demanding because it requires four proton and electron transfers as well as the formation of an oxygen-oxygen bond. Extensive efforts have been made to develop efficient OER catalysts which can catalyze oxygen evolution at low overpotentials. Currently, the most widely used OER catalysts are expensive ruthenium and iridium oxides. Although many alternative catalysts based on earth abundant metal oxides, phosphates, chalcogenides, and molecular catalysts have been suggested, substantial improvement of catalyst activity is still needed. Furthermore, examining the nature of the loaded electrocatalyst and its interaction with the semiconductor are essential for understanding and creating improved efficiency in photoelectrochemical (PEC) water splitting. The source of catalytic improvement of electrocatalyst on semiconductor will be discussed.

Symposium : **MAT1-4**

Synthesis and Application of Multifunctional Nanocatalyst Materials

Room 405+406, THU 16:55

Chair: Sang-II Choi (Kyungpook National University)

Single-crystal 2D heterostructure on wafer scale

Soo Min Kim

Korea Institute of Science and Technology, Korea

Although polycrystalline hexagonal boron nitride (PC-hBN) has been realized, defects and grain boundaries still cause charge scatterings and trap sites, impeding high-performance electronics. Here, we report a method of synthesizing wafer-scale single-crystalline hBN (SC-hBN) monolayer films by chemical vapor deposition. The limited solubility of boron (B) and nitrogen (N) atoms in liquid gold promotes high diffusion of adatoms on the surface of liquid at high temperature to provoke the circular hBN grains. These further evolve into closely packed unimodal grains by means of self-collimation of B and N edges inherited by electrostatic interaction between grains, eventually forming an SC-hBN film on a wafer scale. This SC-hBN film also allows for the synthesis of wafer-scale graphene/hBN heterostructure and single-crystalline tungsten disulfide.

Symposium : **MAT1-5**

Synthesis and Application of Multifunctional Nanocatalyst Materials

Room 405+406, THU 17:20

Chair: Sang-II Choi (Kyungpook National University)

Advanced energy conversion and storage devices using nanostructured materials

Jung Tae Park

Department of Chemical Engineering, Konkuk University, Korea

New materials hold the key to fundamental advances in energy conversion and storage, both of which are vital in order to meet the challenge of global warming and the finite nature of fossil fuels. Nanostructured materials offer unique properties or combinations of properties as electrodes and electrolytes in a range of energy conversion and storage devices. Also, one of the key challenges facing the widespread use and commercialization of promising energy conversion and storage devices (i.e. solar cells, photoelectrochemical cells, electrochemical cells, supercapacitors etc.) is the high cost of the electrode and electrolyte materials and inefficiencies in their assembly and utilization. In this talk, I will present examples of how we are designing nanostructured materials such as self-assembled copolymers, inorganic materials and hybrid templates that can be incorporated into multifunctional composites for high performance energy conversion and storage devices.

Symposium : **MAT2-1**

Controlling Properties of Organic/inorganic Materials for Optoelectronic Devices

Room 405+406, FRI 09:00

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

Organic-Inorganic Hybrid Materials for Advanced Functionality Development in Large Area Electronics

Myung-Gil Kim

Department of Chemistry, Chung-Ang University, Korea

There is increasing demands of material developments for high electrical performance, novel mechanical functionality, high electrical stability, and exotic chemical stability under harsh condition. Although the organic materials and inorganic materials have been investigated with diverse approaches, the combination of these materials as hybrid materials might result synergetic effects for unprecedented properties. To achieve the stabilization and control of the electrical properties in solution-processed amorphous-oxide semiconductors (AOSs) for the realization of cost-effective, high-performance, large-area electronics, we employ a multifunctional organic-semiconductor (OSC)/a solution-processed thin-film hybrid structure.¹ As an electrically active impurity blocking layer, the OSC layer enhances the electrical stability of AOS TFTs by suppressing the adsorption of environmental gas species and copper-ion diffusion. Moreover, charge transfer between the organic interlayer and the AOS allows the fine tuning of the electrical properties and the passivation of the electrical defects in the AOS TFTs. Furthermore, the proper design of organic/inorganic hybrid structure resulted exceptional electrical stability under harsh high energetic proton irradiation, which makes our device promising for aerospace application.² Finally, the unique superlattice structure of hybrid materials resulted exception mechanical stability for flexible electronic applications.³

References

1. G. Kwon, K. Kim, B. D. Choi, J. Roh, C. Lee, Y.-Y. Noh, S.Y. Seo, M.-G. Kim*, C. Kim* *Adv. Mater.*, **29** (2017) 1607055.
2. B. Park, D. Ho, G. Kwon, D. Kim, S. Y. Seo, C. Kim*, M.-G.* Kim *Adv. Funct. Mater.*, **28** (2018) 1802717.
3. L. M. Nhut, K. Kim, K. Baeg, S. K. Park*, M.-G. Kim *In Prepration*.

Symposium : **MAT2-2**

Controlling Properties of Organic/inorganic Materials for Optoelectronic Devices

Room 405+406, FRI 09:25

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

Understanding Solidification of Polythiophene Thin Films during Spin-Coating

Yeong Don Park

Department of Energy and Chemical Engineering, Incheon National University, Korea

Unlike the solvent drop casting, typical film deposition method such as spin-coating, which can be used to produce large-scale homogeneous film, cannot be used to produce ordered structures because of the fast solvent evaporation rate during film formation. In this study with the aim of enhancing the charge transport of polythiophene by promoting molecular ordering, we have developed a casting method via spin-coating time control. By manipulating the spinning time, it is possible to regulate the solvent evaporation rate of solution, which in turn improved the crystallinity of polythiophene thin films. With the short spinning time, the resulting polythiophene thin film adopt a ordered nanowire structures with a field-effect mobility improved by a factor of 10 depending on the spin time. By combining the advantages of the conventional spin-casting and drop-casting methods, we were able to produce semiconducting polymer thin film with high crystallinity and uniformity.

Symposium : **MAT2-3**

Controlling Properties of Organic/inorganic Materials for Optoelectronic Devices

Room 405+406, FRI 10:00

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

Effect of Processing Additives on Organic Photovoltaics: Recent Progress and Future Prospects

Sooncheol Kwon, Kwanghee Lee^{1,*}

Research Institute for Solar and Sustainable Energies (RISE), Gwangju Institute of Science and Technology, Korea

¹*Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

Due to the short diffusion length of approximately 10 nm of an exciton in bulk heterojunction (BHJ) organic solar cells (OSCs) comprising electron donors and acceptors, a formation with well phase-separated nanomorphology in BHJ films has been one of the most important issues in achieving efficient charge separation and extraction in OSCs. By adding a small amount of a high boiling point solvent or molecules to a bulk heterojunction (BHJ) solution, processing additive techniques have recently begun to offer an attractive and efficient method for controlling the nanoscale BHJ morphology of state-of-the-art OSCs with power conversion efficiencies (PCEs) exceeding approximately 11%. However, it remains unknown whether the effect of processing additives can potentially pave the way for the ongoing development of various BHJ components and the commercialization of OSCs. Here, recent progress in understanding and developing the effects of processing additives on OSCs is highlighted. This overview suggests possible guidelines for a wide range of BHJ components with respect to morphological/structural evolution. Furthermore, the rational correlations among processing additives, BHJ components, and fabrication technologies and the performance of high-performance and low-cost OSCs are discussed along with future commercialization prospects.

Symposium : **MAT2-4**

Controlling Properties of Organic/inorganic Materials for Optoelectronic Devices

Room 405+406, FRI 10:25

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

TTA-based Upconversion: Principle and Biophotonic Applications

Jaehyuk Kim

Department of Chemical and Environmental Engineering, Pusan National University, Korea

Upconversion (UC) refers to a photon-frequency amplification process in which the energy absorbed by UC media from two or more incident photons is combined and one photon with higher energy is subsequently emitted, resulting in an anti-Stokes shift. In this presentation, some introductory stories about TTA-UC including basics of the photon energy, mechanisms involved in TTA-UC, achievement and limitation of previous researches will be given first. Then the latest development in our lab – novel vehicle for UC-oil laden hollow mesoporous silica and its biophotonic applications – will be introduced. The details are as follows:

A recyclable, aqueous-phase functioning, and biocompatible photon upconverting system is developed. Hollow mesoporous silica microcapsules (HMSMs) with ordered radial mesochannels were employed, for the first time, as vehicles for the post-encapsulation of oil-phase triplet-triplet annihilation upconversion (TTA-UC), capable of homogeneous suspension in water. In-depth characterization of such upconverting oil-laden HMSMs (UC-HMSMs) showed that the mesoporous silica shells reversibly stabilized the encapsulated UC oil in water to allow efficient upconverted emission, even under aerated conditions. In addition, due to the lipophilic nature of the encapsulated UC oil, UC-HMSMs were found to be actively bound on the surface of human mesenchymal stem cells (hMSCs) without significant cytotoxicity, providing a new concept for integrating TTA-UC and stem-cell therapy. These findings reveal the great promise of UC-HMSMs to serve as ideal vehicles not only for ultralow-power in vivo imaging but also for stem cell labeling to facilitate the tracking of tumor cells in animal models.

Symposium : **MAT3-1**

Material Design and Applications for Artificial Photosynthesis

Room 405+406, FRI 14:30

Chair: Won-Sik Han (Seoul Women's University)

Development of Stable Dye-sensitized Photoelectrosynthesis Cell (DSPEC) for Solar Fuel Production

Kyung-Ryang Wee

Department of Applied Chemistry, Daegu University, Korea

We will introduce an artificial photosynthesis system for solar fuel production from the dye-sensitized photoelectrochemical cell (DSPEC), which is molecular level light absorption and oxidation or/and reduction catalyst approaches. In the DSPEC, the achievement of long-term stability in various pH conditions has long been a central goal of molecular-based solar energy conversion strategies. Here we describe an electrochemically polymerization procedure for preparing chromophore-catalyst assemblies on the nanoparticle metal oxide electrode surfaces for the long-term stable DSPEC system in various aqueous conditions, especially in high pH. Also, the electropolymerization strategy is a simple toolkit for preparing spatially controlled, multicomponent films and surface assemblies having both light harvesting chromophores and catalysts on the metal oxide electrodes. On the nanoparticle metal oxide films as a photoanode, excitation of the assembly with 1 sun (100 mW cm⁻²) illumination in phosphate buffer at pH 7~12 with an applied bias leads to water splitting in a DSPEC with a Pt cathode. Over multiple hour photolysis experiment in high pH condition, electrochemically prepared photoanode shows sustained water splitting with no significant photocurrent decrease. Instability of the surface bound chromophore in its oxidized state in the phosphate buffer leads to a gradual decrease in photocurrent and to the relatively modest faradaic efficiencies. These results indicate that the electropolymerized chromophore-catalyst assembly is a simple toolkit to make stable DSPEC system in various pH conditions for solar fuel production.

Symposium : **MAT3-2**

Material Design and Applications for Artificial Photosynthesis

Room 405+406, FRI 14:55

Chair: Won-Sik Han (Seoul Women's University)

Preparation of single crystal metal foils through colossal grain growth and some of their uses

Sunghwan Jin

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

Polycrystalline metals have randomly oriented crystal grains separated by grain boundaries. In contrast, single crystal metals are composed entirely of one crystal grain without any grain boundaries throughout the sample, and as a result, exhibit properties distinct from polycrystalline metals. Until now, commercial single crystal metals are manufactured by bulk crystal growth processes (such as by the Czochralski or Bridgman methods) but these methods lead to expensive single crystal metals. Here, we present a new technology that can inexpensively convert commercial polycrystalline metal foils into single crystal metal foils. By minimizing contact stresses during the annealing of a metal foil, we discovered colossal growth of grains, resulting in a single crystal metal foil having identical orientation in both the in-plane and out-of-plane directions [1]. We will discuss our method to obtain and to analyze such metal foils, and explain a plausible mechanism for this colossal grain growth. We will also show the growth of single crystal mono- and multi-layer graphenes on single crystal metal foils, and better electrical conduction of single crystal metal foils (a 7% reduction in the room-temperature resistivity of single crystal Cu foils compared to polycrystalline Cu foils) as examples of the applications of such single crystal metal foils. We then speculate on other potential uses of single crystal metal foils including at industrial scale. [1] *Science*, 2018, 362, 1021-1025. Acknowledgements This work was supported by IBS-R019-D1. I thank M. Huang, Y. Kwon, L. Zhang, B. W. Li, S. Oh, J. Dong, D. Luo, M. Biswal, B. V. Cunning, P. V. Bakharev, I. Moon, W. J. Yoo, F. Ding, H. J. Shin, R. S. Ruoff for their great contributions in this work.

Symposium : **MAT3-3**

Material Design and Applications for Artificial Photosynthesis

Room 405+406, FRI 15:30

Chair: Won-Sik Han (Seoul Women's University)

Advantageous Crystalline-Amorphous Phase Boundary in Metal-Metalloid for Electrochemical Water Oxidation

Hyuksu Han

Korea Institute of Industrial Technology, Korea

The development of cost-effective and high-performance electrocatalysts is the primary concern for electrochemical water oxidation applications. Researchers recently reported that the interface between the amorphous layer and crystalline surface plays an important role in enhancing the electrocatalytic activity of transition metal compounds; the high density of the interface between amorphous and crystalline phases should be able to further enhance water oxidation activity of transition metal compounds. In this work, we developed a new and facile strategy for designing high-performance transition metal borides for water splitting by inducing the formation of high density crystalline/amorphous phase boundaries via surface fluorination. Computational simulation was firstly conducted to test our material design principle, followed by experimental verification for optimization. The material design principle proposed in this work is a facile and cost-effective way to considerably enhance the water oxidation activity of metal-metalloids for electrocatalyst applications.

Symposium : **MAT3-4**

Material Design and Applications for Artificial Photosynthesis

Room 405+406, FRI 15:55

Chair: Won-Sik Han (Seoul Women's University)

Highly Selective and Durable Photochemical CO₂ Reduction by Molecular Mn(I) Catalyst Fixed on Particular Dye-Sensitized TiO₂ Platform

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)₃Br (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 (HCOO⁻ versus CO) that surpass the catalytic activities of the 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 persistently produced HCOO⁻ with a >99% selectivity accompanied by a trace amount of CO; the turnover number (TON_{formate}) reached ~250 after 23 h irradiation. The product selectivity (HCOO⁻/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 at low Mn concentration, the Mn-H monomeric mechanism associated with HCOO⁻ formation is dominant, whereas at high Mn concentration, CO is formed via an Mn-Mn dimer mechanism.

Symposium : **ELEC1-1**

New Frontiers in Electrochemistry: Fundamentals and Applications

Room 407+408, THU 15:40

Chair: Byung-Kwon Kim (Sookmyung Women's University)

Diethoxydiethylsilane as a multi-functional organic additive for Ni-rich cathode materials

Taeun Yim

Department of Chemistry, Incheon National University, Korea

Lithium-ion batteries (LIBs) have received considerable attention as the most promising energy storage/conversion system from small- to large-scale devices such as electric vehicles and energy storage system. In this regard, Ni-rich NCM cathode materials ($\text{LiNi}_x\text{Co}_y\text{Mn}_z\text{O}_2$, $x \geq 0.6$) have gained great attention as one of alternative cathode materials in conventional LIBs as they can afford high specific capacity, which allows high energy density of the cell. Nevertheless, poor surface stability of Ni-rich NCM cathode materials should be overcome because it triggers rapid fading of the cell. In this work, we propose silyl group functionalized organic material as 1) a functional additive in the electrolyte or 2) coating-precursor for Ni-rich NCM cathode material in order to decrease fluoride concentration in the cell which causes rapid fading of the cell. Because Si has a high binding affinity with fluoride species, we anticipate that use of DODSi in the cell greatly reduces concentration of fluoride species via chemical scavenging reaction. We confirm that DODSi effectively scavenges fluoride species in the cell via chemical reaction and it allows improved electrochemical performances for 100 cycles.

Symposium : **ELEC1-2**

New Frontiers in Electrochemistry: Fundamentals and Applications

Room 407+408, THU 16:10

Chair: Byung-Kwon Kim (Sookmyung Women's University)

Mechanism of Contact Electrification and Redox Reaction for Au with Polydimethylsiloxane

Seongpil Hwang^{*}, Changsuk Yun¹, Juhyoun Kwak²

Department of Advanced Materials Chemistry, Korea University, Korea

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

²*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

The investigation on the static charge generation by contact electrification between Au and polydimethylsiloxane (PDMS) and the redox reaction by the static charge in the aqueous phase will be presented to reveal the mechanism of contact electrification and redox reaction which may be applied to mechanical-to-chemical energy harvesting. First topic is the mechanism of contact electrification. There are two controversial mechanism of electron transfer and ion migration. The static charge distribution on the equipotential Au was probed through Kelvin probe force microscopy (KPFM) in air after the contact with patterned PDMS to reveal what happens during the contact. Second, the redox reaction by the charged Au was electrochemically monitored using open circuit potential (OCP), stripping voltammetry, and copper underpotential deposition (UPD). All electrochemical experiments consistently resulted in the reduction of the reactant by the charged Au within the highly dielectric water media. The suggested behavior of contacted Au in water will be introduced.

Symposium : **ELEC1-3**

New Frontiers in Electrochemistry: Fundamentals and Applications

Room 407+408, THU 16:40

Chair: Byung-Kwon Kim (Sookmyung Women's University)

Electrophoretic Deposition for the Development of Bio-compatible Hydrogel-CNT Composites

Young Soo Joung

Department of Mechanical Systems Engineering, Sookmyung Women's University, Korea

In this work we present a novel method to fabricate composite nanomaterials in hydrogel membranes using electrophoretic deposition (EPD) at the interface of two immiscible liquids. Hydrogels have been employed for bio-materials due to their outstanding bio-compatibility, high porosity, and notable swelling capabilities. Further, conductive hydrogel films have been investigated because they can provide a critical methodology to sense and diagnose biological systems or be used in energy storage applications. Here, we propose a novel process employing electrophoretic deposition (EPD) at the interface of immiscible liquids to create composite hydrogel films. EPD uses electrophoresis to deposit thin films of nanoparticles normally onto conductive solid-substrates. However, during interfacial EPD, nanoparticles such as carbon nanotubes (CNTs) electro-migrate to an oil/water interface, where polymer cross-linking is induced to form composite hydrogel membranes. The key aspect of this method is that polymerization occurs away from a solid substrate while surrounded by both polar and nonpolar media, allowing for the integration of CNTs or other nanoparticles into the hydrogel. Properties of the composite hydrogel films are controlled by the deposition parameters and polymerization time, facilitating mass production without the need for complex machinery. This fabrication method is cost-effective and scalable for composite hydrogels with tunable electrical, mechanical, and biological properties. Potential applications include fabrication of doped hydrogels for drug delivery and conductive hydrogels for biological sensing.

Symposium : **ELEC1-4**

New Frontiers in Electrochemistry: Fundamentals and Applications

Room 407+408, THU 17:10

Chair: Byung-Kwon Kim (Sookmyung Women's University)

Fundamental Understanding of Electroosmosis Is a Key for Developing Drug Delivery Pump

Woonsup Shin^{*}, Junyeong Kang¹

Department of Chemistry / Department of Fusion Bio, Sogang University, Korea

¹Department of Chemistry, Sogang University, Korea

Electrochemistry is known to be a key transducing technology between chemical energy and electrical energy. Electroosmosis is a phenomenon which the fluid moves upon applying electric field through capillary or porous ceramic membrane. This is a rare example where electrochemistry is utilized for a mechanical transducer. Electroosmotic pumps are the simplest one, consisting of two electrodes separated by a porous membrane, but its practical use has been hindered by the use of platinum electrode. On platinum the pumped solution keeps being electrolyzed to produce O₂ from anode and H₂ from the cathode and the bubbles are easily trapped in the membrane to make the flow irregular. Even the co-production of O₂ and H₂ makes the system unsafe in the closed loop. The use of electrochemical reaction such as Ag/Ag₂O could substitute the reactions on the platinum electrode to operate the pump non-gassing with higher efficiency. It also enabled the pump battery-operable. The pump is now currently being used to develop drug pumps such as insulin patch pump and implantable morphine pump.

Symposium : **ELEC2-1**

Beyond Batteries: Understanding New Types of Energy Storage Technology

Room 303, FRI 09:00

Chair: Inho Nam (Chung-Ang University)

Development of Non-Precious Metal Electrocatalysts Based on Mo-Compounds for Electrochemical Hydrogen Production

Duck Hyun Youn

Department of Chemical Engineering, Kangwon National University, Korea

Development of efficient electrocatalysts for hydrogen evolution reaction (HER) with earth-abundant, non-precious materials is crucial for practical large-scale hydrogen production from electrochemical water splitting powered by renewable energy sources. Molybdenum compounds (Mo-compounds) are attracting great attention recently as a promising replacement for Platinum. Here we synthesized molybdenum carbide, nitride, and sulfide nanocrystals on CNT-graphene hybrid support via modified urea-glass route and their electrochemical activities for hydrogen evolution reaction were systematically investigated. By changing the amount of urea or replacing urea with thiourea, it was possible to control the final phases of the products from nitride, carbide to sulfide. Among the prepared catalysts, Mo₂C/CNT-graphene (Mo₂C/CNT-GR) showed the highest activity for hydrogen evolution reaction (HER) with small overpotential of 62 mV and Tafel slope of 58 mV/dec as well as an excellent stability in acid media. The performance represents one of the best among recently reported Mo-based electrocatalysts. Vastly improved electron transfer characteristics by incorporating CNT-graphene hybrid and low hydrogen binding energy compared to the others are mainly responsible for the excellent activity.

Symposium : **ELEC2-2**

Beyond Batteries: Understanding New Types of Energy Storage Technology

Room 303, FRI 09:20

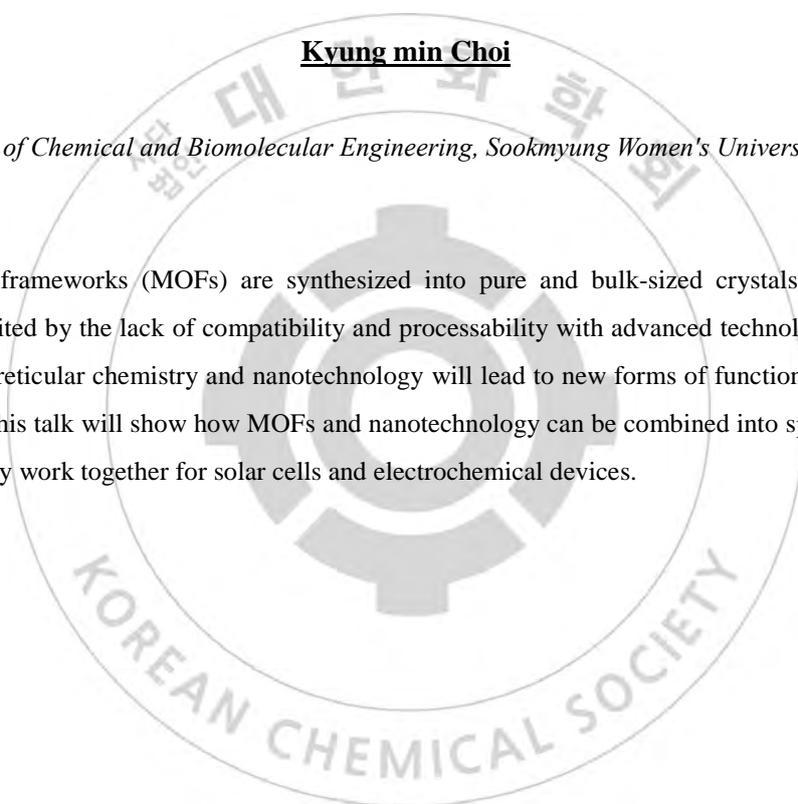
Chair: Inho Nam (Chung-Ang University)

Nanocrystalline Metal-Organic Frameworks for Electrical Applications

Kyung min Choi

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

Metal-organic frameworks (MOFs) are synthesized into pure and bulk-sized crystals, and thus their usability is limited by the lack of compatibility and processability 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 nanotechnology can be combined into special constructs and successfully work together for solar cells and electrochemical devices.



Symposium : **ELEC2-3**

Beyond Batteries: Understanding New Types of Energy Storage Technology

Room 303, FRI 09:50

Chair: Inho Nam (Chung-Ang University)

Prussian Blue open-framework structure for energy storage and harvesting applications

Hyun-Wook Lee

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

Prussian Blue and its analogues (PBAs) have gained great attention due to their interesting properties originating from their flexibility in structure and synthetic methods, allowing a large degree of structural and chemical tunability. PBAs can be prepared by bottom-up assembly of molecular precursors via the formation of continuous chemical bonding between transition metal ions and ligand molecules. These cyanide ligands can enable the long-range charge transport with abundant CN triple bonds that can provide free electrons for electrical conduction. Due to such flexibility in their design and resultant properties, they can have a wide variety of applications including energy storage, harvesting, and catalytic applications. In this talk, I will introduce low-vacancy, sodium manganese hexacyanomanganate (MnHCMn) as a viable cathode material for SIBs. The as-synthesized MnHCMn has nonlinear Mn–N≡C–Mn bonds and containing eight large interstitial sites occupied by Na⁺ ions. Here, I discovered a novel mechanism wherein small lattice distortions allow for the unprecedented storage of 50% more sodium cations than in the undistorted case. Due to the minimal hysteresis in the galvanostatic charge/discharge curves of the electrochemical cell using Prussian Blue open-framework structures, a different approach is to explore thermodynamic cycles as is common in thermomechanical engines. The thermogalvanic effect, the dependence of an electrode's electrochemical potential on temperature, can be used for such cycles. In the second part of my talk, the electrochemical thermodynamic cycle for thermal energy harvesting will be introduced. By utilizing novel electrode materials, this system can achieve very high efficiencies at low-temperature ranges.

Symposium : **ELEC2-4**

Beyond Batteries: Understanding New Types of Energy Storage Technology

Room 303, FRI 10:10

Chair: Inho Nam (Chung-Ang University)

Self-assembly of bio-piezoelectric materials for energy harvesters

Juhyuck Lee

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

Piezoelectric materials are excellent generators of clean energy as they can harvest the ubiquitous vibrational and mechanical forces. Recently, many natural biomaterials (e.g., amino acids, peptides and proteins) that can be synthesized in an environmentally friendly method have been shown to have piezoelectric properties. Particularly, strong piezoresponse on the diphenylalanine (FF) and M13 bacteriophage has been reported. However, the difficulty of fabricating scalable unidirectionally oriented and polarized structures of those materials has been a major impediment to the realization of a strong piezoelectric energy harvesters. In this present, I will show a novel strategy to synthesize large-scale aligned self-assembly bio-piezoelectric materials. The orientation and polarization directions of these materials were controlled using self-assembly nature. Furthermore, the bio-piezoelectric materials based energy harvesters were developed.

Symposium : **ELEC2-5**

Beyond Batteries: Understanding New Types of Energy Storage Technology

Room 303, FRI 10:30

Chair: Inho Nam (Chung-Ang University)

Operando Raman microscopy for redox mechanism in organic cathode materials

Joonhee Moon

Advanced Nano-Surface Research Group, Korea Basic Science Institute, Korea

Rechargeable lithium-ion-batteries are widely used in various application, such as portable devices, bio-medical implants and electric vehicles due to their high energy and power density. However, current lithium-ion batteries based on inorganic materials have nearly reached their ceiling with respect to storage capability. Therefore, breakthroughs in new energy storage system that can surpass the current performance barrier should be brought about in a timely manner. Recently, many researchers have been made to identify organic molecules and polymers for rechargeable batteries. Here, we introduce Raman microspectroscopy installed at Advanced Nano-Surface Research Group in Korea Basic Science Institute (KBSI) which is especially set up in glove box to measure various materials without air exposure, which can exhibit a sample from another surface contamination when exposure to atmosphere. Additionally, we designed and fabricated two types of electrochemical cells developed for studying organic cathode materials during battery operation. This approach simultaneously characterizes phase transition and facilitates uncovering the relationships between surface structure and activity during battery operation. This result provides a method for visualizing chemical structure of phase transition and the changed surface morphology.

Symposium : **EDU-1**

Current Trends in Chemistry Education

Room 204, THU 15:40

Chair: Aeran Choi (Ewha Womans University)

Curriculum of the secondary chemistry teachers' training colleges, is it good?

Jongseok Park

Department of Chemistry Education, Kyungpook National University, Korea

The training of secondary school chemistry teachers is carried out by various institutions, but the curriculum of the teachers' training colleges that are required to be completed is nearly the same. This is because the Ministry of Education has designated the required courses. In particular, the view of the pre-service teachers is a very limited due to the teacher certification examination, regardless of whether they have taken various courses such as major and liberal arts during four years of college. While mentioning the 4th industrial revolution and nurturing human resources to prepare for the future society, but the old education curriculum and the teacher certification examination are becoming obstacles for the pre-service teachers to teach such talents. Therefore, I would like to examine the present curriculum of secondary school chemistry teachers and the contents of the teacher certification examination focusing on the field of chemistry education, and to suggest what should be improved by identifying problems.

Symposium : **EDU-2**

Current Trends in Chemistry Education

Room 204, THU 16:10

Chair: Aeran Choi (Ewha Womans University)

Chemistry Teacher's Professional Development and Secondary School Chemistry Teacher Appointment Examination

HyunJu Park

Faculty of Science Education, Chosun University, Korea

There is a secondary school teacher appointment examination. The national exams is designed to assess the professions of pre-service chemistry teacher. This study conducts an item analysis of the chemistry education questions in the national exams of 2014-2019. The frequency of the chemistry education questions was examined by year, sub-field, and question format. The validity and appropriateness of questions of examination is very important. Inaccuracy, lack of authenticity, the limited number of questions, and/or the area of questioning were pointed out as problems of the national examination. The chemistry education questions from the exam of 2019 appear to be more difficult than the previous ones because the exam extends over topics that are not familiar to examinees and does not clarify the unfamiliar terms used in the questions. It is also shown that chemistry education in the current secondary school teacher education program is not likely to cover the knowledge required by the current recruitment exam, suggesting the need for change in the program or the exam. And I asked a few chemistry teacher whether the questions of the national examination is good enough to evaluate the competencies as a chemistry teacher.

Symposium : **EDU-3**

Current Trends in Chemistry Education

Room 204, THU 16:50

Chair: Aeran Choi (Ewha Womans University)

long term observation of general chemistry education for undergraduate students

Jung Yun Do

Department of Chemical Education, Pusan National University, Korea

New technologies based on chemistry have been accumulated as outcome of social needs, leading to quantitative and qualitative growth in basic science. Fortunately, there is still no change in fundamental knowledge required for students who are about to study chemistry at college and concrete basic contents encountered on textbooks for general chemistry is good hand at education. The books provide the introduction of wide areas of chemistry composing of more than 20 chapters including some history and recent attractive events and usually reviewed throughout and speedy in two semesters. Several specified chapters arranged in the rear can be skipped in general education course such as nucleus chemistry, organic and bio-organic chemistry, and inorganic chemistry in spite of significance in chemistry, chemistry related science and engineering. Equilibrium-related chapters need to be compressed. Whole chapters are not necessary for every student when considering satisfaction and comprehension. The selection of the contents is essential for providing effective education of general chemistry and considered especially for a class consisting of students with different experience and learning from various curriculums of high school. It's no wonder that supplementary materials such as short video and photographs exhibiting related experimental evidences improve the chemistry education. These supplementary data are better to be given by KCS or authentic educational institution.

Symposium : **ENVR-1**

Research Trends in Emerging Contaminants

Room 203, THU 15:40

Chair: Yu Sik Hwang (Korea Institute of Toxicology)

Five W and one H of the regulatory research trend in nanomaterials

Byung-tae Lee

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

Researchers in all fields of engineering and science understand nanomaterials as materials smaller than 1 μ m. Among them, especially nanotechnology researchers refer to substances smaller than 100nm as nanomaterial. Though it is generally defined based on its size, but from an institutional perspective for chemical safety management, it is distinguished from non-nanomaterials with more complex criteria such as number-based size distribution fraction of nano-sized particle in the product. The study of nanomaterial risks has been going on for more than a decade. Nanomaterial is not a new chemical, but a new classification system depending on the properties of the chemical. When a chemical exists in a finite form that exhibits a certain physically apparent size under certain conditions, we can define it as a nanomaterial or a non-nanomaterial. In terms of regulation, applying the management policy of chemicals to nanomaterial is a very complex issue that requires significant changes to the classification system of existing chemicals. Due to this importance, the specified safety regulation on nanomaterials has yet to be implemented, even though a substantial number of scientific and regulatory studies have been carried out. In December 2018 the European Union finally passed a revision of REACH which includes nanomaterials, and a related registration and evaluation of nanomaterials will begin in 2020. The U.S. and Canada, prior to registration and evaluation of chemicals, had implemented a reporting rule to investigate the current state of manufacture and use of nanomaterials. In this presentation, the research trends in nanomaterials will be explained from the institutional perspective of chemical safety management through a 5W1H way. "Why" suggests the need for institutional management of nanomaterials. "What" compares the scientific and legal definitions of nanomaterial and the differences by country. 'Where' shows the major uses of nanomaterial so far. 'When' describes the timing and main content of regulatory management of nanomaterial in major countries. 'Who' looks at stakeholders' interests in nanomaterial management and conflicts with each other's. 'How' describes the framework of nanomaterial safety management. Finally, the regulatory roadmap is suggested for the implementation of nanomaterial in the chemical safety management system.

Symposium : **ENVR-2**

Research Trends in Emerging Contaminants

Room 203, THU 16:10

Chair: Yu Sik Hwang (Korea Institute of Toxicology)

Risks from biocidal active ingredients in consumer products

Jung-Hwan Kwon

Div of Environ Sci & Ecol Engr, Korea University, Korea

Humidifier disinfectant disaster in 2011 invoked the importance of safe management of chemicals in consumer products. Biocidal active ingredients are being added to many chemical products used in our daily lives for various purposes. Although the new regulation on these chemicals (Act on the safe management of consumer chemical products and biocides) has been enacted this year in Korea, the scientific decision support systems needs to be refined during the grace period of the law. In this overview presentation, schemes of the risk and safety assessment methodology used for scientific decision of those products in regulatory context are introduced with an emphasis on biocidal products. Scientific decision support system in general benchmarks systems developed in US and Europe. However, it is of urgent needs to refine inhalation risk assessment methodology for various consumer products because inhalation dosimetry and exposure assessment models used in other countries are also based on very limited amount of experimental evidences.

Symposium : **ENVR-3**

Research Trends in Emerging Contaminants

Room 203, THU 16:50

Chair: Yu Sik Hwang (Korea Institute of Toxicology)

Characteristic Occurrence and Fates of Emerging Contaminants in Korean Water Environment

Jeong-Eun Oh

Department of Environmental Engineering, Pusan National University, Korea

As the industrial development, more than 100,000 kinds of chemicals are being distributed globally and over 2,000 kinds of new chemicals are produced every year. These chemicals are used for variety of applications in everyday life and industry such as pharmaceuticals, cosmetics, pesticides and surfactants etc. Among these chemicals, PPCPs (pharmaceuticals and personal care products), commonly used for the prevention and treatment of diseases of humans are now regarded as emerging chemicals and reported their wide detection in water environment. Besides PPCPs, Perfluoroalkyl substances (PFASs) that have been widely used in multiple industrial applications such as water repellent on clothing, leather, photolithographic film and surface tension lowering agent are also drawing an big attention due to their toxicity and frequent detection in environment, especially in drinking water. Therefore, in this study, we investigated the various emerging contaminants like PFASs and PPCPs in Korean water environment to assess their characteristic occurrence patterns. In addition, the spatial and seasonal variation in water environment and the removal efficiency of these chemicals in WTPs (water treatment plants) was examined. All the target chemicals were analyzed by HPLC-MSMS, a high-performance liquid chromatography connected to a mass spectrometer in multiple reaction monitoring (MRM) and The detailed results will be presented in the conference.

Symposium : **ENVR-4**

Research Trends in Emerging Contaminants

Room 203, THU 17:20

Chair: Yu Sik Hwang (Korea Institute of Toxicology)

Suspect and non-target screening using LC-HRMS for identification and prioritization of emerging contaminants

Junho Jeon

Department of Environmental Engineering, Changwon National University, Korea

In EU, environmental quality standard directive along with water frame directive established a watch list mechanism to support the prioritization of emerging contaminants. The prioritizing processes mainly include risk assessment and monitoring data abundance/quality check. For successful management of emerging contaminants, research parties providing reliable monitoring data are mandatory to support the update and review of the watch list. Advanced analytical techniques can detect contaminants occurring at trace levels. In addition, highly sensitive and selective analytical instruments and the associated screening approach such as suspect and nontarget screening methods enable identifications of unknown/newly occurring contaminants which are of strong candidates for the list in the future. For a preferred example of the parties, NORMAN, network of laboratories and research centres sharing not only monitoring data, but also newly developed analytical methods, has significantly contributed to the prioritization process by providing reliable data on occurrences and concentration of emerging pollutants. The prioritization system with watch list and the relevant association supporting the whole process in EU are benchmarkable for the management of CECs occurring in watersheds, Korea

Symposium : **KCS1-1**

[NFEC] Leading Researcher, Supporting Research Equipment Policy

Room 103+104, WED 15:00

Chair: Dong Woo Kim (NFEC)

An introduction of R&D budget investment efficiency policy and system of national research facilities & equipment

Myeongho Yoon

MSIT, Korea

In this presentation, we will introduce the support system and revision items related to the efficiency improvement policy of national R&D budget, which is recently promoted by the government, and help to understand the research field. We will aim to improve policies centered on researchers. First, the government operates the national research facilities & equipment deliberate system. It deliberates the feasibility of purchasing R&D facilities & equipment when allocating or adjusting its budgets that is deployed with R&D budget. This subject is intended to explain to researchers the national R&D investment deliberation system, and to help them understand it. Second, the National R&D Innovation Plan, which was announced in July 2018, selected 'project management of large research infrastructure' as a project task, referring to the need for systematic and professional management system of large research infrastructure that is the basis for R&D. This is because large-scale government funding is required to build large research infrastructure. Accordingly, the government has prepared guidelines for comprehensive project management for large research infrastructure, and the PM system is applied to projects aimed at establishing research infrastructure in the next year. Third, there is a difficulty in stable operation of large research facility equipment built with a large budget. Accordingly, the Ministry of Science and Technology has prepared guidelines for operating expenses for large research facilities equipment. In this presentation, we will explain operation support policy for large research facility equipment with total construction cost of over 10 billion won.

Symposium : **KCS1-2**

[NFEC] Leading Researcher, Supporting Research Equipment Policy

Room 103+104, WED 15:50

Chair: Dong Woo Kim (NFEC)

Research infrastructure support policy for the innovative research performance (Of the researcher, by the researcher, for the researcher)

Kyoungmi Lee^{*}, Bitnam Hwang^{*}

NFEC, Korea Basic Science Institute, Korea

NFEC(National Research Facilities and Equipment Center) supports the establishment of a full-time operation and utilization system for promoting R&D performance and sharing research infrastructures based on 「the 2nd Advancement plan」 . This year, we launched a pilot project, which helps collect the underutilized research equipment in the universities and create core facilities by research area. Accordingly, we selected 3 universities and funded expenses for transfer, setup, repair and upgrade of the equipment, enhancing the utilization of the research equipment and the R&D capacity in the universities. Also, as MSIT and MOE will adopt and launch Core-Facility Project, we will be able to enhance the utilization of the research facilities and equipment as well as the R&D capacity. Meanwhile, by improving the existing policy, which focuses on purchase and management, we have introduced policy suggestions such as 'Research facilities and equipment cost pooling system' which will be implemented from Sep. 2019.

Symposium : **KCS1-3**

[NFEC] Leading Researcher, Supporting Research Equipment Policy

Room 103+104, WED 16:30

Chair: Dong Woo Kim (NFEC)

An introduction of research equipment education platform to strengthen research capacity

Insu Seo

National Research Facilities and Equipment Center, Korea Basic Science Institute, Korea

Today, research facilities and equipment(F&E) are becoming an important means of driving the development of science and technology, and the government is pursuing various support policies based on the "The 2nd Research F&E Advancement Plan". As part of this effort, NFEC is supporting ZEUS F&E portals to support joint use of research equipment and improve research productivity. In 2019, the ZEUS Education Menu will be newly established to support researchers' research capacity enhancement. Following : (Equipment) Training book, training information, manuals, operation video, site map, community, intellectual services. In addition, the ZEUS point system will be introduced to support researcher participation in education programs and purchase of educational books. This support policy will be enforced in June 2019.

Symposium : **KCS2-1**

Future Technology for a Super-Connected Boundless Society [The 14th Story of Future IT Technology with
DONGWOO FINE-CHEM]

Room 404, THU 16:00

Chair: Myunsoo Kim (DONGWOO FINE-CHEM)

IoT technology in extreme environment

Haksun Kim

Ulsan National Institute of Science and Technology, Korea

In this seminar I will introduce new communication technology that used surface transfer wave guessing magnetic force.

We found new phenomenon to propagate information through metal surface when we use TE mode wave generator.

IoT solutions provide by wired or wireless method. But we don't have underground or in the water or shield environments without wire.

We developed surface wave generator and automatic tuning circuits for best efficient power transfer condition through metal surface.

IoT terminal and pier to pier communication, and total extreme condition solution using our new technology have been developed.

But there is no solutions for high temperature packaging material in furnace or spaceship yet that can change high temperature to electric voltage.

I hope IoT service to cover all of the world under extreme circumstances for enhanced safety.

Symposium : **KCS2-2**

Future Technology for a Super-Connected Boundless Society [The 14th Story of Future IT Technology with
DONGWOO FINE-CHEM]

Room 404, THU 17:00

Chair: Myunsoo Kim (DONGWOO FINE-CHEM)

The Key Materials and Process Technology for Next Generation Display

Junho Song

Korean University, Korea

Following the cathode ray tube (CRT), TFT LCD flat panel displays started production in 1993 and became the main display for 25 years. Since then, OLEDs that can be flexibly used have rapidly spread around smartphone application, and they have become a premium product for large displays such as TVs. However, recently, various technologies such as OLED-based quantum dots, transparent OLEDs, foldable displays, rollerable and scalable displays as well as u-LEDs have been developing due to the quality of ultra-high colors and needs for various display applications. In this presentation, the next Generation display technology would be introduced and the key materials and process technologies required based on their requirement would be discussed.

Symposium : **KCS3-1**

NRF Presentation on the Basic Research Fund

Room 203, FRI 09:00

Chair: Duk-Young Jung (Sungkyunkwan University)

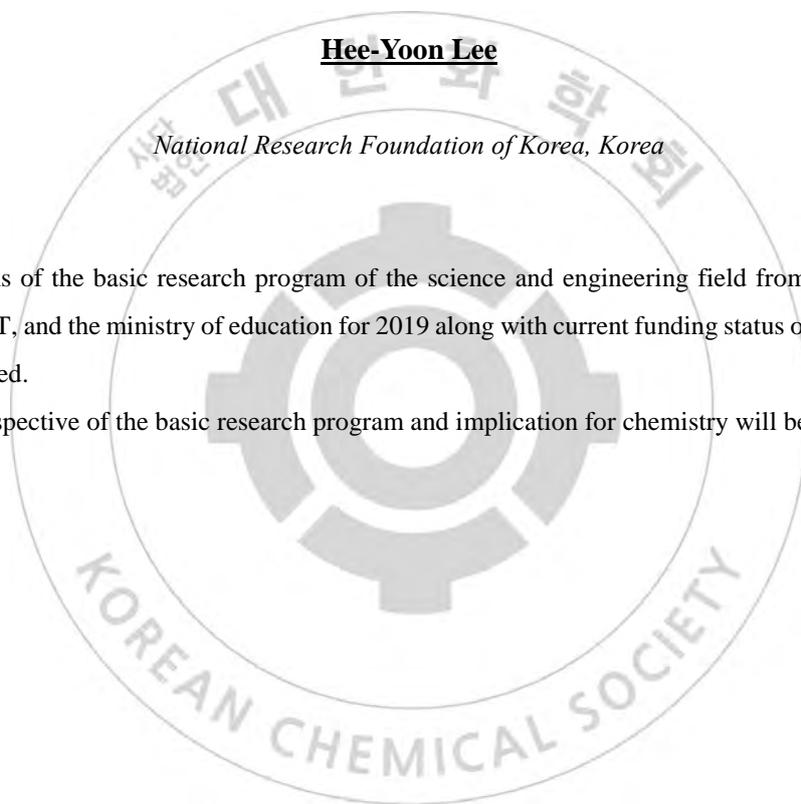
Operation Plans of the Basic Research Programme of the Science and Engineering Field in 2019 and beyond; Implication for Chemistry

Hee-Yoon Lee

National Research Foundation of Korea, Korea

Operation plans of the basic research program of the science and engineering field from the ministry of science and ICT, and the ministry of education for 2019 along with current funding status of chemistry field will be presented.

The future perspective of the basic research program and implication for chemistry will be discussed.



Symposium : **KCS5-1**

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

Room 404, FRI 09:00

Chair: Ik-Mo Lee (Inha University)

What To Think Prior To Research and Development in Laboratory

Sunyoung Bae

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

Research and development associated with sciences require time to start and conduct projects through various processes. Laboratory safety should be considered even before starting the experiments. 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 prior to research. 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. The real case of laboratory hazard risk assessment will be introduced to the graduate research students, the principal investigators, and other related personnel for having an opportunity to think the necessary processes prior to experiment and to understand each role toward a culture of safety.

Keywords: Laboratory safety, Research and Development Safety Analysis, Hazard, Ris

Symposium : **KCS5-2**

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

Room 404, FRI 09:40

Chair: Ik-Mo Lee (Inha University)

Risk Assessment System and Laboratory Accreditation

Young Man Kim

Advanced Analysis Center, Korea Institute of Science and Technology, Korea

Researches in universities and research institutes are becoming more dangerous than those in industries because recent experiments have been done under diverse and complicated conditions. As a result, many accidents have occurred continuously and lab workers are more anxious about the safety in the lab. In response of this situation, government enforces more strict measures for the safe management of hazardous materials.

In this presentation, the enhancement of safe consciousness in the lab is aimed to ensure the safe of lab workers. Several ways to become a better organization in the management of environment and safety will be proposed by establishing the preliminary risk analysis of hazardous factors and self-control safe management system.

Symposium : **KCS5-3**

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

Room 404, FRI 10:20

Chair: Ik-Mo Lee (Inha University)

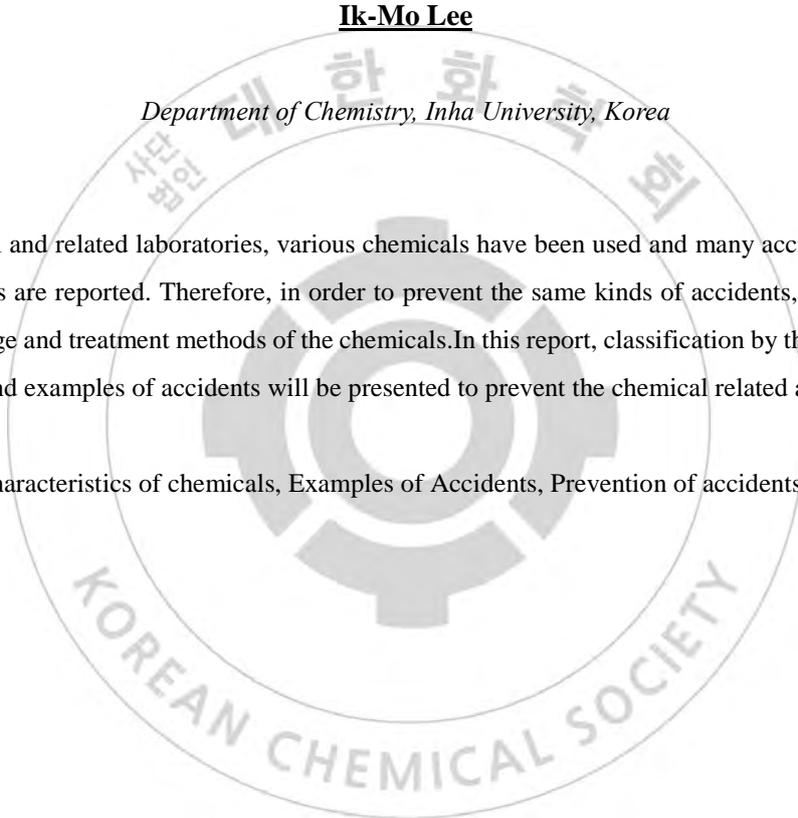
Characteristics of Chemicals and Examples of Accidents

Ik-Mo Lee

Department of Chemistry, Inha University, Korea

In the chemical and related laboratories, various chemicals have been used and many accidents caused by these chemicals are reported. Therefore, in order to prevent the same kinds of accidents, it is essential to know the storage and treatment methods of the chemicals. In this report, classification by the characteristics of chemicals and examples of accidents will be presented to prevent the chemical related accidents.

Key Words: Characteristics of chemicals, Examples of Accidents, Prevention of accidents



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

Oral Presentation for Young Polymer Scientists

Room 403, THU 09:00

Chair: Jeewoo Lim (Kyung Hee University)

Living Anionic Polymerization of Furfuryl methacrylate

Kyeongsoo Shin, Myung-Han Yoon^{1,*}, Jae suk Lee^{2,*}

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

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

²*Department of Advanced Materials Engineering, Gwangju Institute of Science and Technology, Korea*

Furfuryl methacrylate (FMA) is an interesting material because of the presence of the furan group as the reactive diene functionality. However, FMA cannot be polymerized by the conventional radical polymerization due to the side reaction, where radicals attack the reactive furfuryl group in the polymer and in the monomer. As a result, FMA becomes insoluble and gelled polymers even at low conversion, due to excessive chain transfer. Many researchers have developed different methods to prevent this side reaction, which are Atomic Transfer Radical Polymerization (ATRP) and (Reversible Addition-Fragmentation chain Transfer) RAFT. These methods were the success for FMA polymerization without insoluble and gelled polymer. However, the method of anionic polymerization did not go unreported for controlled polymerization which is a narrow polydispersity index (PDI) and controlled molecular weight. So, we try to polymerize the FMA having narrow PDI and controlled molecular weight via anionic polymerization.

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 09:12

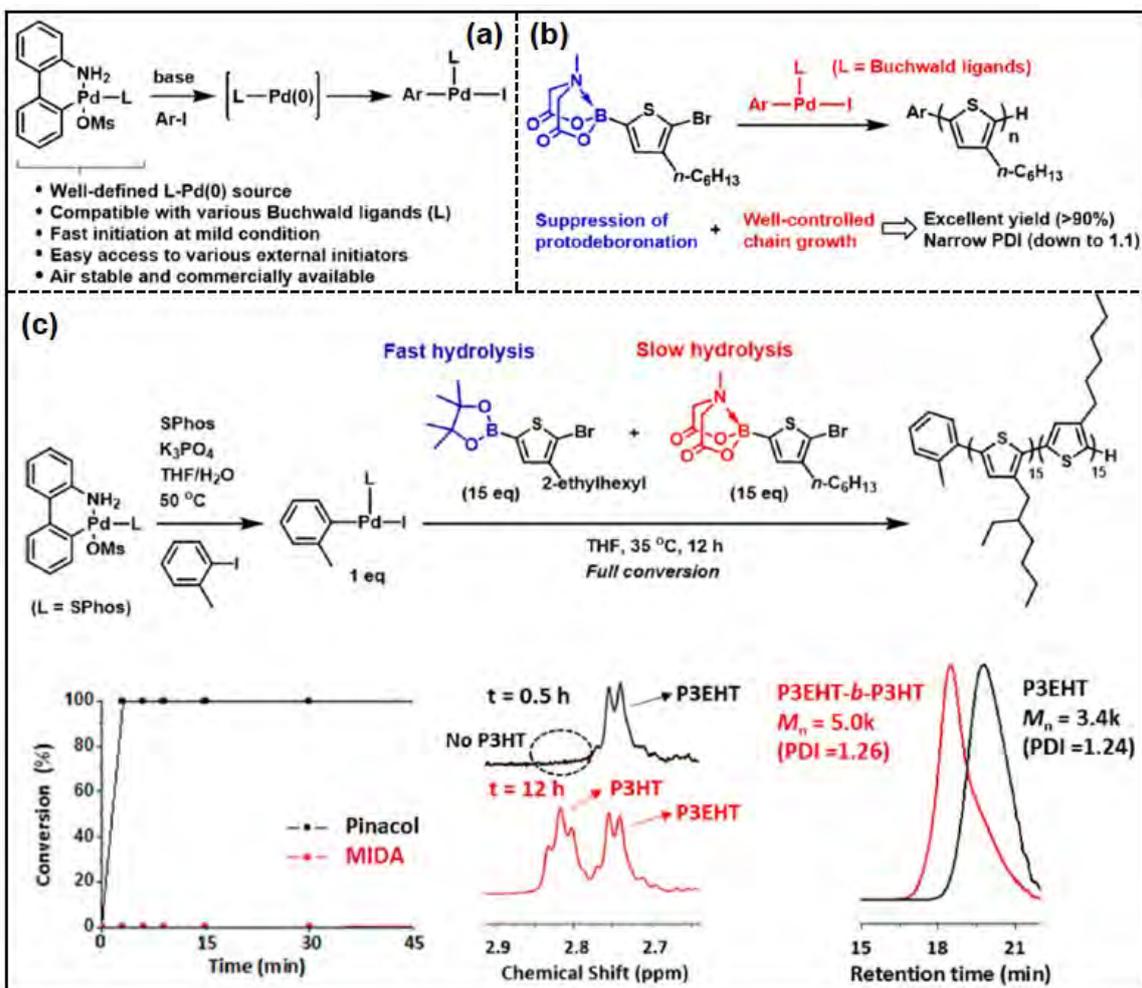
Chair: Jeewoo Lim (Kyung Hee University)

A Rational Design of Highly Controlled Suzuki-Miyaura Catalyst-Transfer Polycondensation for Synthesis of Regioregular Poly(3-alkylthiophene)s and Their Block Copolymers

Jaeho Lee, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

Introduction Kumada catalyst-transfer polycondensation (KCTP) method is the most widely used method to synthesize conjugated polymers, which have been intensively investigated due to their intriguing applications to optoelectronic devices, in a chain-growth manner. However, using moisture-sensitive Grignard reagents gave practical disadvantages. On the other hand, air-/moisture-stable boronates have been used for Suzuki-Miyaura catalyst-transfer polycondensation (SCTP), which makes SCTP as a promising alternative for KCTP. Despite these advantages, the use of a less efficient catalyst system and the competing protodeboronation of heterocyclic boronate monomer limited the wide application of SCTP. Herein, we report a highly controlled SCTP of 3-alkylthiophenes using Buchwald dialkylbiarylphosphine Pd G3 precatalysts and *N*-methylimidodiacetic (MIDA)-boronates. **Results and Discussion** RuPhos and SPhos Pd G3 precatalysts were identified as excellent catalyst systems for the catalyst-transfer process by optimizing a small molecule model reaction. SCTP was tested using pinacolboronate thiophene monomer, but controlled poly(3-hexylthiophene) (P3HT) was obtained for a low DP only. To improve the control, slowly hydrolyzed MIDA-boronate thiophene monomer was introduced. As a result, P3HT and P3EHT (up to 17.6 kg/mol) were prepared with excellent control, narrow dispersity (90%). Detailed mechanistic studies using NMR and MALDI-TOF spectroscopy revealed that both catalyst-transfer of Buchwald catalysts and slow hydrolysis of MIDA-boronate were crucial to achieve successful SCTP of P3HT. Furthermore, block copolymers were prepared via SCTP by both sequential monomer addition and one-shot methods.



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

Oral Presentation for Young Polymer Scientists

Room 403, THU 09:24

Chair: Jeewoo Lim (Kyung Hee University)

Discovery of Highly Efficient Organic Photoredox catalysts for Visible Light Driven Atom Transfer Radical Polymerization

Varun Singh, Min Sang Kwon^{1,*}

Materials science and Engineering, Ulsan National Institute of Science and Technology, Korea

¹*Division of Advanced Materials Engineering, Ulsan National Institute of Science and Technology, Korea*

Organocatalyzed atom transfer radical polymerization (O-ATRP) offers an attractive variant to traditional ATRP as it eliminates the concern associated with transition metal contamination in final polymer products which otherwise hinder their application in biomedical and electronics applications. However, in the current scenario high catalyst loadings are required to control the molecular weight of polymers and the limited monomer scope is a major obstacle in efficient use of organic photoredox catalysts (OPCs). In this talk, I will present a systematic computer aided design strategy to discover new photocatalysts which overcome these challenges. Specifically, one of the discovered OPCs controls polymerization of methyl methacrylate at sub-ppm catalyst loadings, 0.5 ppm, thus enabling a direct use of polymers without catalyst-removal process and, another OPC having high excited state reducing power facilitate the polymerization of challenging nonacrylic monomer like styrene which is not possible using existing OPCs. We envision that our design strategy can provide first step towards rational development of photocatalysts for polymer and organic synthesis.

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 09:36

Chair: Jeewoo Lim (Kyung Hee University)

Multi-Responsive Dynamic covalent Hydrazone Supramolecular Polymers

Kyung-su Kim, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Stimuli-responsive polymeric systems are of considerable interest due to their potential applications in environment-adaptive technologies such as smart surfaces. Traditionally, such systems can be constructed either by dynamic non-covalent (supramolecular) or dynamic covalent chemistry, but the use of both chemistries in one system offers unique opportunities for structural diversity and various controllability. Herein, we report that hydrazone-pyridinium conjugates, which can be dynamically exchanged by transimination, can be assembled into one-dimensional wires by direct intermolecular interactions (without metal-ion coordination). The self-assembly process can be controlled not only by dynamic covalent chemistry, but also by pH adjustment. The hydrazone-pyridinium conjugates are transformed to merocyanine-type dyes of distinctive negative solvatochromism via deprotonation, which affects their self-assembly. Such a dual control of the dynamic molecular assembly will provide a way to develop diverse smart materials with multi-stimuli-responsiveness

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 09:48

Chair: Jeewoo Lim (Kyung Hee University)

Phase behavior and ion transport properties of acid-bearing block copolymer containing ionic liquids

Ha Young Jung, Moon Jeong Park^{1,*}

Chemistry, Pohang University of Science and Technology, Korea

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

Ion-containing block copolymers, consisting of mechanically robust hydrophobic block and ion-conducting hydrophilic block, are of interest for polymer electrolyte membranes given that microphase separation behavior of block copolymers offers simultaneous achievement of high mechanical strength and high ionic conductivity. Ion-conducting block is commonly prepared by modifying polymer backbones with protogenic moieties. Most widely investigated systems are sulfonated polymers owing to the easy synthetic steps and high dissociation degree of proton. Other protogenic groups such as phosphonic acid group have also been attracted great interest, enabling self-dissociation of proton under dry conditions. In this study, we study the polymers based on bis(sulfonyl) imide groups, which have low pKa value than that of sulfonic acid counterpart. Morphology and ion transport properties of bis(sulfonyl) imide-tethered block copolymers were investigated with a focus on the role of protogenic groups in determining proton transport efficiency along nanoscale ionic phases. Especially, with the introduction of ionic liquids, dissimilar thermodynamic interactions of ionic liquids with protogenic groups of polymers led to markedly different phase behavior of resultant block copolymer electrolytes

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 10:00

Chair: Jeewoo Lim (Kyung Hee University)

Structural Modification of Sulfur-based Polymer for Broad Application

Jaecil Park, Myung-Han Yoon*

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

It is well known that elemental sulfur is the promising material for upcoming generation. Although various methods such as physical or chemical modification were developed to use elemental sulfur, limited structure was reported. In this research, poly (sulfur-r-1,3 Diisopropenylbenzene) was synthesized via inverse vulcanization in solvent. LDI-ToF was used to measure molecular weight and the number of residual double bond were calculated using $^1\text{H-NMR}$ and EA. Average molecular weight is about 1200 g/mol and 0.5 double bonds per molecule remain unreacted. Through this functional group, photo-patterning was demonstrated by irradiating UV lamp (415 nm) for 20 min. Furthermore, copolymerization with another (meth)acrylate monomer was carried out by using P(S-DIB) as a macro chain transfer agent. It is expected that structural modification extends applicable field of the sulfur-based polymer.

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 10:12

Chair: Jeewoo Lim (Kyung Hee University)

Formation of uniform one-dimensional- and two-dimensional-nanostructures from fluorescent semiconducting polymers with orthorhombic crystalline orientation

Sanghee Yang, Tae-Lim Choi^{1,*}

Chemistry, Seoul National University, Korea

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

Owing to the potential applications of nanostructures consisted of conjugated polymers (CP), the self-assembly of the CP is taking the spotlight in the supramolecular chemistry field. Also, one of the most important requirements for the applications, the precise control of the shape and size of the structures is essential. Fortunately, through interesting crystallization-driven self-assembly (CDSA) for well-known crystalline polymers reported by Manners group first, we have successfully controlled the size of various multidimensional nanostructures. However, only a few examples of living one-dimensional (1D)- or two-dimensional (2D)-CDSA for crystallizable CPs have been reported in spite of their high potential as functional optoelectronic materials. Based on our early investigations on the living cyclopolymerization, we designed new crystalline P1 homopolymer containing a fluorene moiety with bulky neohexyl groups on monomer units. To prepare fully conjugated block copolymer (BCP) including P1 as the second block, we polymerized soluble first block (P2) followed by polymerizing P1. To fully investigate the structural properties of the structures, we used various microscopes and X-ray diffraction analysis. As results, we achieved to form two-dimensional (2D)-nanosheets from the P1 homopolymer with the tunable height. By expanding the P1 to the BCP (P2-b-P1), we also succeeded in the formation of rigid 1D-nanoribbons with tunable length and width via 1D-CDSA. More recently, we have succeeded in producing the uniform monolayer 2D-nanosheets from the 2D-CDSA of P1 for the 2D-rectangular micelles by blending the crystallizable polymers. Those unique fluorescent semiconducting nanostructures with tunable shapes are potentially useful in optoelectronic applications.

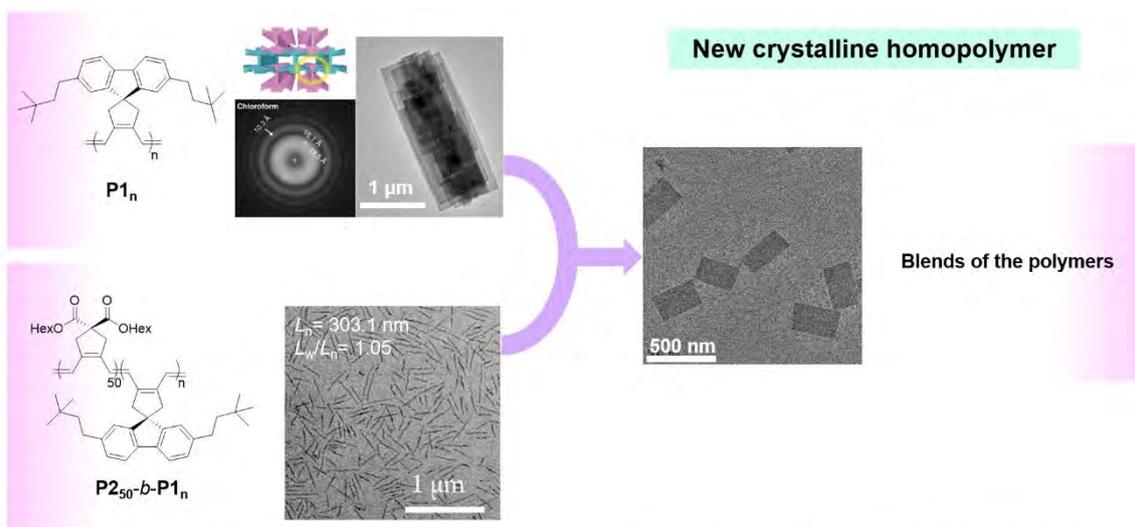


Figure 1. Summary of various 1D- and 2D-nanostructures *via* controlled self-assembly of simple CPs



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

Oral Presentation for Young Polymer Scientists

Room 403, THU 10:24

Chair: Jeewoo Lim (Kyung Hee University)

Polymer Aggregation Control of NDI-Based Conjugated Polymer with Improved Electrical Connection through Backbone Fluorination

Seung Un Ryu, Yelim Choi, Taehyun Kim, Dohyun Kim¹, Taiho Park^{2,*}

Pohang University of Science and Technology, Korea

¹*Chemical engineering, Pohang University of Science and Technology, Korea*

²*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

Naphthalene diimide (NDI)-based conjugated polymer with bithiophene (BT) or dithienylethene (TVT) are widely used in organic electronic devices as n-type materials and, in general, these can form large crystal domains through NDI-driven self-assembly. However, they still have limitations on improving electron transport mainly due to the lack of electrical connection between crystal domains. An interconnected network of weakly ordered aggregates with mixed orientation could provide an effective approach to increase the electron mobility of a polymer. We demonstrate the feasibility of approach using NDI-based polymer with TVT having fluorine in the 3-position instead of hydrogen (FTVT). FTVT unit enhances intermolecular interactions between polymer chains, leading to robust aggregation. This aggregation suppresses NDI-driven self-assembly to produce interconnected aggregates with short-range order and affords a reinforced film morphology at elevated temperature. This microstructure resulted in improved μ of transistor devices by lowering energetic disorder as well as continuous electrical connection at different annealing temperatures.

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 10:36

Chair: Jeewoo Lim (Kyung Hee University)

Sulfonated mesoporous membrane with high ion permselectivity for vanadium redox flow batteries

Choongseop Jeon, Myungeun Seo^{1,*}

*graduate school of nanoscience and technology, Korea Advanced Institute of Science and Technology,
Korea*

¹*Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology,
Korea*

Mesoporous membranes with well-controlled pore size are useful for size-exclusive separation, where substances only smaller than the pore can traverse across the membrane. In a vanadium redox flow battery (VRFB), cation permselectivity providing facile proton transport and suppressed vanadium cross-over is one of the most important issues to ensure long cyclability without loss of voltage efficiency. We show that sulfonated mesoporous membranes synthesized via polymerization-induced microphase separation almost exclude vanadium cross-over when the pore size is below at 4 nm. Proton conductivity is retained because of facilitated hopping process along the sulfonated pore surface. VRFB cell data suggests higher efficiency and slower decrement in discharge Q compared to Nafion 212, demonstrating promise of this approach.

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

Oral Presentation for Young Polymer Scientists

Room 403, THU 10:48

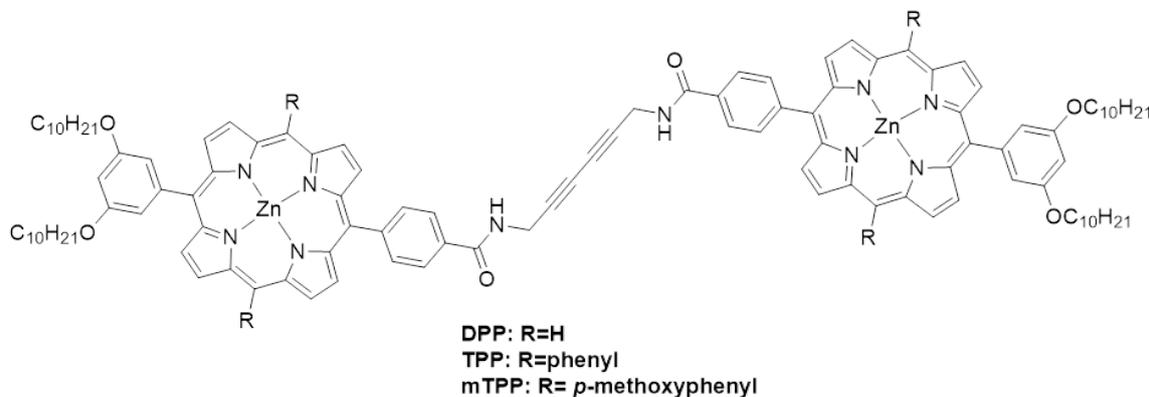
Chair: Jeewoo Lim (Kyung Hee University)

Helicity control of achiral bisporphyrin-based supramolecular polymer through chiral-auxiliary approach

Hosoowi Lee, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Recently, the control of supramolecular polymerization process has attracted attention to many researchers. We designed a series of bisporphyrin derivatives (**DPP**, **TPP**, **mTPP**), composed of two zinc porphyrin units bridged by amide groups and diacetylene moiety with long alkyl side chains. All three bisporphyrins were self-assembled in methylcyclohexane (MCH) at low temperature (273 K) through hydrogen bonding and π - π stacking. Unlike **DPP** and **mTPP**, **TPP** show distinct different aggregation mode upon preparation method; UV/Vis absorption spectra show that J-aggregates and H-aggregates were formed from fast and slow cooling of hot MCH solution, respectively. UV/Vis absorption spectral changes of **TPP** J-aggregate clearly exhibited the transformation from J-aggregate to H-aggregates. The transformation process of J-aggregates was visualized through atomic force microscopy (AFM) and these AFM images show helical assembled nanofibers of **TPP**. Through chiral-auxiliary approaches to this transformation process, we can control the helicity of aggregated nanohelices.



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

Oral Presentation for Young Polymer Scientists

Room 403, THU 11:00

Chair: Jeewoo Lim (Kyung Hee University)

Generation of luminescent silver nanodots in the presence of amino silane and sodium polyacrylate

Sungmoon Choi, Yanlu Zhao, Junhua Yu*

Department of Chemical Education, Seoul National University, Korea

Amino silane has been introduced to suppress the further growth of luminescent silver clusters (silver nanodots) to non-luminescent silver nanoparticles in the stabilization of the just-reduced silver clusters with sodium polyacrylate (PAA). The pre-treatment of silver ions with amino silanes before mixing the silver and PAA significantly improved the yield of luminescent silver clusters/silver nanodots. The roles of the silver, silane, and sodium polyacrylate in the generation of such chromophores are still vague. We found that silver ions and the PAA chain formed chromophoric complexes in the aqueous solution. However, silver nanodots were generated only after chemical reduction. The silane with two or three amino groups promoted the generation of silver nanodots, but an increase in hydrophobicity of the silane, i.e., flanked by a single amino group, stimulated the formation of near-IR silver nanodot emitters. Nevertheless, the absorption spectrum of the reaction mixture did not superimpose in shape with the excitation spectrum of the silver nanodot, suggesting that there were multiple-species that caused strong absorptions in the visible and near-IR region. The pH of the solution strongly influenced the generation and stability of silver nanodots. Silver nanodots were generated efficiently when the reaction pH was between 6 and 8, whereas the already-formed silver nanodots were stable at the pH values between 6 and 10, suggesting that disruption of the silver nanodot protection by competitive species in the solution was slowed down due to the chelate effect of multiple bonding from the polymer chain. Our results suggest that the microenvironment of silver nanodots influences strongly the properties of silver nanodots.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:00

Chair: Minyoung Yoon (Gachon University)

Synthesis of Iridium (III) complexes including bis-NHC ligands : applying to amine to alcohol conversion

Yeon Joo Cheong, Hye-Young Jang^{1,*}

Department of Energy System Research, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Electron-rich N-heterocyclic carbene (NHC) ligands have many advantages in synthesizing stable transition metal catalyst complexes. Because of the strong sigma donation ability of NHC ligands, metal ions strongly coordinate to NHC ligands, leading the formation of metal, which are oxygen and moisture stable. Bidentate NHCs behave like hemilabile ligands and can easily generate vacant sites in the metal complex. In addition, NHC is easy to introduce additional functional groups. NHC complexes with alcohol, alkoxide, phenoxide, ether, N-heteroaryl, oxazoline, amino and amido have been reported. These additional groups mediate interactions between the ligand and the reactants or between the ligand and the catalyst, which increases the reaction rate and selectivity. In this study, we have made various structurally modified Iridium (III) bis-NHC complexes, which are employed in the conversion of amines to alcohols.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:10

Chair: Minyoung Yoon (Gachon University)

Rational Design and Construction of Hierarchical Superstructures Using Shape-persistent Organic Cages: Porphyrin Box-based Metallosupramolecular Assemblies

**Younghoon Kim, Jaehyoung Koo, In-Chul Hwang¹, Rahul Dev Mukhopadhyay¹, Kimoon
Kim***

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

¹*Center for Self-assembly and Complexity (CSC), Institute for Basic Science (IBS), Korea*

A novel approach to constructing hierarchical superstructures made up of porphyrin box (PB), a porous organic cage, is presented. We have previously reported a series of rationally designed porous organic cages, the porphyrin boxes (PBs), which consist of square-shaped porphyrin and triangular-shaped triamine subunits. The truncated cubic-shaped geometry and six porphyrin faces of the PBs prompted us to explore metallated PBs as pre-made and atomically-precise organic building units to construct hierarchical superstructures linked by properly designed ditopic bridging ligands. Using this approach, we obtained two- and three-dimensional PB-based superstructures (PSS), and found that there is an optimum range of the linker length for the construction of PSSs. The hierarchical structures were confirmed by single-crystal X-ray diffraction analysis. The PSSs have a protein-like large unit cell (>40 Å) with a spacious void volume (62%) and larger extrinsic surface area compared to that of the parent PBs, which can be exploited for selective encapsulation of guest molecules, interior functionalization, catalysis etc. As a proof-of-concept, we demonstrated that singlet oxygen-induced synthesis of a natural product, juglone, is more efficiently catalyzed in presence of PSS-1 than by its constituent component Zn-PB.^{1,2}References¹Kim, Y.; Koo, J.; Hwang, I.-C.; Mukhopadhyay, R. D.; Hong, S.; Yoo, J.; Dar, A. A.; Kim, I.; Moon, D.; Shin, T. J.; Ko, Y. H.; Kim, K. J. *Am.Chem. Soc.* 2018, 140, 14547-14551.²Mukhopadhyay, R. D.;§ Kim, Y.;§ Koo, J.;§ Kim, K. *Acc. Chem. Res.* 2018, 51, 2730-2738.

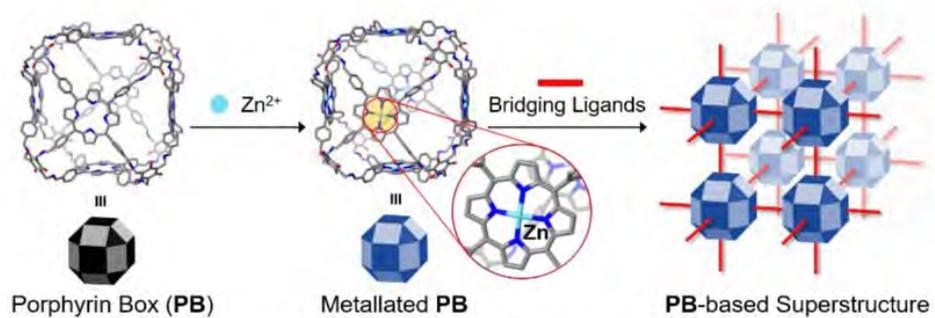


Figure 1. The schematic illustration of the approach adopted for the construction of PB-based superstructures.



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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:20

Chair: Minyoung Yoon (Gachon University)

Chemical Strategies to Modify Amyloidogenic Peptides by Iridium(III) Complexes: Coordination and Photo-Induced Oxidation

Juhye Kang, Jung Seung Nam, Tae-Hyuk Kwon¹, Mi Hee Lim^{2,*}

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

¹*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

²*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Amyloidogenic peptides are considered central pathological contributors towards neurodegeneration as observed in neurodegenerative disorders [e.g., amyloid- β ($A\beta$) peptides in Alzheimer's disease (AD)]; however, their roles in the pathologies of the diseases have not been fully elucidated since they are a challenging target to be studied due to their heterogeneous nature and intrinsically disordered structure. Chemical approaches to modify amyloidogenic peptides would be valuable in advancing our molecular-level understanding of their involvement in neurodegeneration. In this presentation, effective chemical strategies for modifications of $A\beta$ peptides implemented by a single Ir(III) complex in a photo-dependent manner will be presented and discussed. Such peptide variations can be achieved by our rationally designed Ir(III) complexes leading to the significant modulation of the aggregation pathways of $A\beta_{40}$ and $A\beta_{42}$, as well as the production of toxic $A\beta$ species. Overall, we demonstrate chemical tactics for modifications of amyloidogenic peptides in an effective and manageable manner utilizing the coordination capacities and photophysical properties of transition metal complexes.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:30

Chair: Minyoung Yoon (Gachon University)

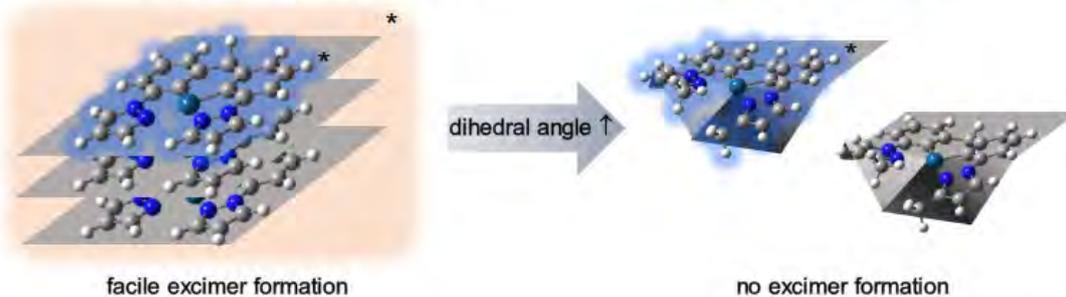
Toward Deep Blue Electrophosphorescence from Cyclometalated Pt(II) Complexes

Yu Kyung Moon, Youngmin You*, Kim Jang-Joo^{1,*}

Division of Chemical Advanced Materials, Ewha Womans University, Korea

¹*Division of Material Engineering, Seoul National University, Korea*

Square-planar d^8 Pt(II) complexes constitute important dopants for organic light-emitting devices (OLEDs). However, blue electrophosphorescence from Pt(II) complexes remains underdeveloped. This lag originates from the deterioration of color purity due to the formation of excimers. One appealing approach to addressing this challenge would be breaking planarity of a Pt(II) complex using a tetradentate ligand having large steric hindrance. To achieve this goal, we designed and synthesized three Pt(II) complexes having tetradentate ligands with varied methyl substituents, di(3-(pyrazol-1-yl)phenyl)methide (for PtSN1), di(3-(4-methylpyrazol-1-yl)phenyl)methide (for PtSN2), and di(3-(3-methylpyrazol-1-yl)phenyl)methide (for PtSN3). The complexes displayed blue phosphorescence emission with peak wavelengths of 438-442 nm in dilute solutions. PtSN3 retained its inherent blue emission when doped in mCBP films at a concentration of 8 wt %, whereas PtSN1 and PtSN2 showed dominant excimer emissions at the same doping concentrations. The equilibrium constant (K) for the formation and dissociation of excimers were determined to be as large as $1.17 \times 10^4 \text{ M}^{-1}$ and $0.69 \times 10^4 \text{ M}^{-1}$ for PtSN1 and PtSN2, respectively. OLEDs were fabricated using the PtSN compounds as dopants, which yielded the maximum external quantum efficiencies of 14.1% (PtSN1), 13.7% (PtSN2), and 8.6% (PtSN3). The inferior performance of the PtSN2 device was ascribed to a low photoluminescence quantum yields (0.33 vs 0.57 (PtSN1) or 0.58 (PtSN2)), suggesting a trade-off relationship between the color purity and efficiencies.



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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:40

Chair: Minyoung Yoon (Gachon University)

A New Class of Bifunctional One-component Catalysts for the Synthesis of Cyclic Carbonates

Yoseph Kim, Seol Ryu¹, Youngjo Kim*

Department of Chemistry, Chungbuk National University, Korea

¹*Department of Chemistry, Chosun University, Korea*

At this seminar, I want to talk about a new class of halide-free and bifunctional one-component catalysts for the coupling of CO₂ with epoxides. These catalysts do not need halide-based additives or tethered salts attached to ligand when used for this coupling reaction. As the halide-free and bifunctional one-component catalysts, nonionic and monomeric tetracarbonylchromium(0), tetracarbonylmolybdenum(0), and tetracarbonyltungsten(0) complexes chelated by modified ethylenediamines were chosen. In addition, we will directly compare the catalytic activity of simple mixture of M(CO)₆ (M = Cr, Mo, and W) and the modified ethylenediamines with the catalytic activity of the synthesized tetracarbonyl metal complexes precoordinated to the corresponding modified ethylenediamines. We found that increasing the number of methyl substituents on the nitrogen atoms of the ethylenediamine derivatives as well as the chromium metal center in the metal carbonyl complex significantly enhanced the catalytic activity. Furthermore, we will show that various terminal and internal epoxides were easily converted into the corresponding cyclic carbonates using our system. Finally, calculations based on density functional theory were also carried out to elucidate the mechanism of the coupling reaction.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 09:50

Chair: Minyoung Yoon (Gachon University)

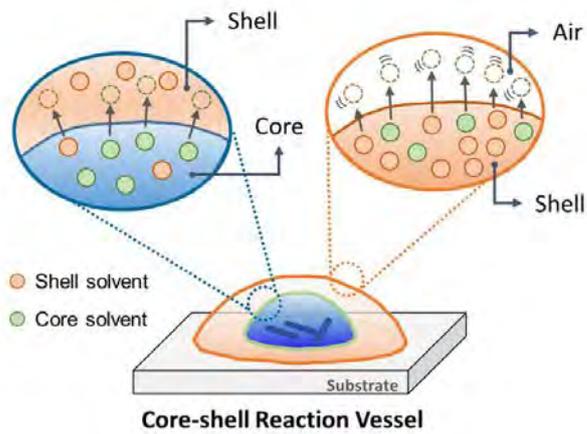
Crystallization of Organic Molecules by a modified Drop-drying Method Using Binary Solvent Core-shell Droplet

Yoolim Ahn, Yohwan Park, Jinyoung Koo, Hee Cheul Choi*

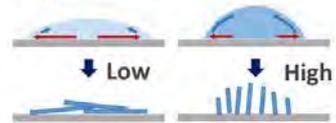
Department of Chemistry, Pohang University of Science and Technology, Korea

In this presentation, we present a core-shell drop-drying (CSDD) method that employs spontaneous formation of the core-shell droplet for the efficient growth of organic molecular crystals. A drop-drying method is one of the simplest crystallization methods that allows a direct growth of organic molecular crystals on a solid substrate. Despite the advantages of drop-drying process, the practical applications to organic molecular crystals are very limited due to the poor area-selectivity and low crystallinity of the resulting crystals. To overcome these limitations, a modified drop-drying method that employs a droplet-in-droplet system is newly designed. The droplet-in-droplet system has an inner core that droplet enables area selective growth with suppressed coffee-ring effect, and an outer shell droplet that provides enough crystallization time to form well-defined facets. Using this concept, well-defined ribbon-shaped methylene blue crystals were successfully grown from methanol/methylene core-shell droplets with significantly diminished coffee-ring effect, while the conventional mono-solvent system using methanol solution did not succeed. The crystallization mechanism of CSDD revealed that the diffusion and evaporation of solvents at the core-shell and shell-air interfaces were key factors for suppressing coffee-ring effect. In addition, the CSDD method provides the diversity of crystal in terms of sizes and growth direction by changing the droplet condition, such as concentration or solvent volume ratio. We expect that this method will not only contribute the in-depth understanding of crystallization mechanism in binary solvent systems but also expand the usage of drop-drying method to develop organic molecular crystals that could be applied in various fields.

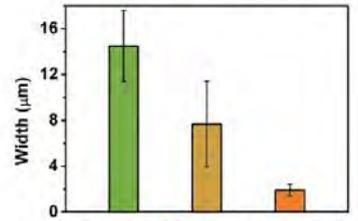
Droplet-in-Droplet System



Precursor Concentration



Growth direction control



Crystal width control



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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:00

Chair: Minyoung Yoon (Gachon University)

Building Principles of Meta-MOF (Metal-Organic Framework)

Eunji Jin, Dongwook Kim¹, Hosoo Lee², Woo-Dong Jang³, Myoung Soo Lah, Seung Kyu Min*, Wonyoung Choe*

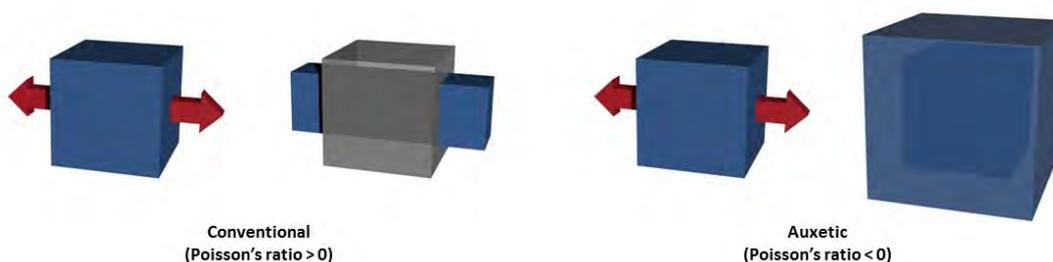
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²*Department of Chemistry, College of Science, Korea*

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Mechanical metamaterials, artificial materials with counter-intuitive properties such as a negative Poisson's ratio, not exhibited by conventional materials that is found in nature. Unusual properties of metamaterials are obtained from structural geometry, not their composition. Rational design of mechanical metamaterials at the micro- and macroscale is interesting as found novel geometries. However, incorporating movable building blocks inside solids, thereby enabling us to manipulate the mechanical movement at the molecular scale, has been a difficult task. Here we report a metal-organic framework, self-assembled from a porphyrin linker and a new type of Zn-based secondary building unit, acted as a joint in hinged cube tessellation. We show that this material is indeed mechanical metamaterial, exhibiting auxetic behaviour through detailed structural analysis and theoretical calculation. This work demonstrates that the topology of the framework and flexible hinges inside the structure are intimately related to the mechanical properties of the material, providing a guideline for the rational design of mechanically responsive metal-organic frameworks.



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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:10

Chair: Minyoung Yoon (Gachon University)

Structure-Thermopower Relationships Achieved with Large-Area Thermoelectric Molecular Junctions

Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Studies of thermopower in molecular junctions permit access to the atomic-detailed energy topography across junctions and how thermopower is associated with chemical structure of the active molecular components inside junctions. In this presentation, we show liquid metal-based thermoelectric junction technique and structure-thermopower relationships established with the technique. Cone-shaped liquid Ga-In alloy (EgIn) microelectrode allows us to achieve high yields of working junctions and thus statistically sufficient thermoelectric data sets. Using this new technique, we tested the dependence of thermopower on the length of molecules with and without π -electrons: that is, oligophenylene and n-alkane monothiolates chemisorbed on gold substrates. Our results reveal that the length dependence of thermopower predominantly depends on the presence and absence of π -conjugation. The change of Seebeck coefficient as a function of molecular length is opposite for the oligophenylene and n-alkane backbones : as the length of molecules increases, Seebeck coefficient increases and decreases for oligophenylene and n-alkane backbones, respectively. These findings are consistent with previous results in literature. More interestingly, thermoelectric junction measurements over n-alkane monothiolates indicate that the decrease rate of Seebeck coefficient changes at n-undecanethiolate (SC11) from -0.60 to -0.034. We discuss the origin of this observation based on metal-induced gap states (MIGS), which have been theoretically proposed (and not experimentally proven yet) in self-assembled monolayers on gold.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:20

Chair: Minyoung Yoon (Gachon University)

Zintl Phase Thermoelectric Material with the *n*-type dopant: $\text{Ca}_{5-x-y}\text{Yb}_x\text{RE}_y\text{Al}_2\text{Sb}_6$

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 $A_5M_2Pn_6$ ($A = \text{Ca, Sr, Eu, Yb}$; $M = \text{Al, Ga, In}$) 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 $\text{Ca}_{3.21(1)}\text{Yb}_{1.65}\text{Pr}_{0.15}\text{Al}_2\text{Sb}_6$ was successfully synthesized by arc-melting, and its crystal structure was characterized by both powder and single-crystal X-ray diffractions. It has been 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 compound adopts the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type structure whereas the Ba-rich compound adopts the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type structure. Nevertheless, the Ca-rich rare-earth containing title compound adopted the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type with the orthorhombic space group $Pbam$ ($Z=2$, Pearson Code $oP26$) after the initial arc-melting and the post heat treatment transformed to the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type structure. According to the SXRD result, only one cationic site contains the *n*-type dopant RE^{3+} with a particular site-preference. In addition, the thermoelectric property measurement implies that the initial $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type compound was *p*-type, while the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type compound was the *n*-type TE material. To understand the interesting TE property transition from the *p*-type to the *n*-type character, a series of theoretical calculations using three hypothetical models by tight-binding linear muffin-tin orbital method were performed, and the results were thoroughly analyzed.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:30

Chair: Minyoung Yoon (Gachon University)

Potential applications of imidazolium-based Metal-Organic Frameworks

Jaechul Lee, Chong Yang Chuah¹, Kimoon Kim*, Minyoung Yoon^{2,*}, Daewoon Lim^{3,*}, Tae-Hyun Bae^{1,*}, Eunsung Lee*

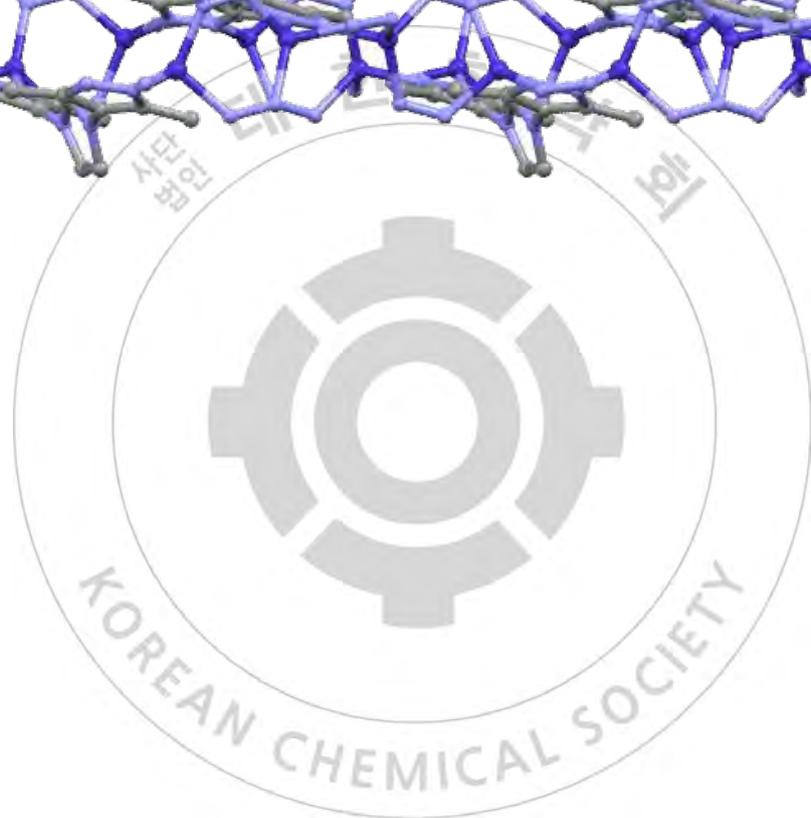
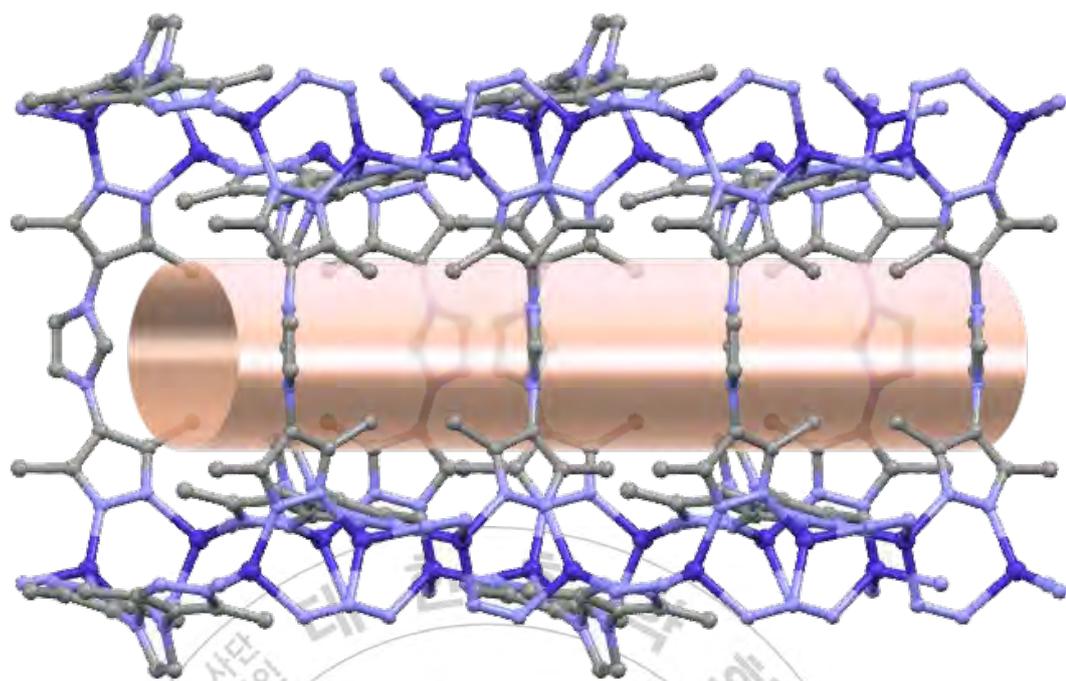
Department of Chemistry, Pohang University of Science and Technology, Korea

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²*Department of Nano Chemistry, Gachon University Global Campus, Korea*

³*Department of Chemistry, Kyoto University, Japan*

Metal-organic frameworks (MOFs) have attracted great interest due to their potential applications such as catalysis, gas storage, and separation of molecules. Organic linkers bearing imidazolium functional group have been emerged as a building unit for constructing several MOFs. However, there is a little study on the utilization of imidazolium functionality in MOFs for various applications. In this research, we designed a new imidazolium ligand with pyrazolate as a metal binding sites and synthesized cobalt based 3D MOF from the ligand. The potential applications of the MOF (**JCM-1**) have been studied. In this presentation, 1) hydrocarbon separation, 2) ammonia capture and 3) proton conduction applications will be introduced.



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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:40

Chair: Minyoung Yoon (Gachon University)

3d-transition metal doped Ir-based octahedral nanocages as efficient electrocatalysts for the oxygen evolution reaction

Taehyun Kwon, Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nanocatalysts with hollow interior have received enormous attention due to their high electrocatalytic activity toward water splitting. Iridium (Ir)-based hollow nanostructures, in particular, have shown a great potential as stable electrocatalysts for the oxygen evolution reaction (OER) under acidic condition, which is the rate determining step for overall water splitting reaction. We have recently discovered that the cobalt (Co) doping to the Ir oxide material phase greatly boosts the catalytic efficiency of oxygen evolution reaction by otherwise not very active Ir oxide, derived from IrCu phase. We further found that other 3d-transition metal elements such as Mn and Zn like Co could also enhance the catalytic efficiency of Ir oxide phase. In this seminar, we will describe the role of these transition metal dopants in the catalytic Ir oxide phase and point out the future direction of OER catalyst design.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 10:50

Chair: Minyoung Yoon (Gachon University)

Structure and Reactivity of a Mononuclear Nonheme Manganese(III)-Iodosylarene Complex

Donghyun Jeong, Jaeheung Cho*

Emerging Materials Science, DGIST, Korea

Transition metal-iodosylarene complexes have been proposed to be key intermediates in the catalytic cycles of metal catalysts with iodosylarene. We report the first X-ray crystal structure and spec-troscopic characterization of a mononuclear nonheme manganese(III)-iodosylarene complex with a tetradentate macrocyclic ligand, $[\text{Mn}^{\text{III}}(\text{TBDAP})(\text{OIPh})(\text{OH})]^{2+}$ (**2**). The manganese(III)-iodosylarene complex is capable of conducting various oxidation reactions with organic substrates, such as C-H bond activation, sulfoxidation and epoxidation. Kinetic studies including isotope labeling experiments and Hammett correlation demonstrate the electrophilic character on the Mn-iodosylarene adduct. This novel intermediate would be prominently valuable for expanding the chemistry of transition metal catalysts.

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

Oral Presentation of Young Inorganic Chemists

Room 401+402, THU 11:00

Chair: Minyoung Yoon (Gachon University)

Metal Effect with Regioisomeric Controls of Ligands on Metal-Organic Frameworks

Hyeon Bin Ha, Dopil Kim, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs) are organic-inorganic hybrid materials consisting of metal clusters (or ions) and multitopic organic ligands. MOFs generally have three-dimensional frameworks with permanent porosity, and sometimes they show flexible frameworks. The flexibility of MOFs (i.e., structural changes of MOF frameworks) is changed by external stimuli such as pressure, guest molecular contact, solvent, etc. Recently, we have revealed that the position of functional groups and electronic density of ligands are also directly related with the flexibility changes of MOFs. Among the various combinations of functionalities, only NH₂-Cl, NH₂-Br, NH₂-OMe, OMe-OMe displayed the flexibility changes by the position of functional groups (i.e., regioisomeric of functional group).¹⁻³

Herein, we have expanded our regioisomerism research to metal effect on MOFs. Using *para*- and *ortho*-NH₂-Cl functionalized ligands, we have successfully prepared three MOFs with different metal salts (cobalt, copper, and zinc) but with identical structures. Their structural analysis along with gas adsorption changes will be discussed in this presentation.

References

1. Kim, M.; Boissonault, J. A.; Dau, P. V; Cohen, S. M. *Angew. Chem. Int. Ed.* **2011**, *50*, 12193.
2. Hahm, H.; Yoo, K.; Ha, H.; Kim, M. *Inorg. Chem.* **2016**, *55*, 7576.
3. Ha, H.; Hahm, H.; Jwa, D. G.; Yoo, K.; Park, M. H.; Yoon, M.; Kim, Y.; Kim, M. *CrystEngComm*, **2017**, *19*, 5361.

Oral Presentation : **PHYS1.O-1**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:00

Chair: Ilsun Yoon (Chungnam National University)

A simple and accessible microscopic magnetic field mapping techniques using exciplex-based magnetosensing fluorophore: One- and Two-photon excitation

Dongkyum Kim, Hohjai Lee^{1,*}

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

¹*Chemistry, Gwangju Institute of Science and Technology, Korea*

We developed the simple and accessible fluorescence microscopic imaging system for mapping magnetic field. The system includes a fluorescent indicator, pyrene-(CH₂)₁₂-O-(CH₂)₂-*N,N*-dimethylaniline respond to magnetic field. Upon photo-excitation, the indicator forms an excited complex (exciplex) or spin-correlated radical ion pairs (RIP) via excited state quenching. The amount of exciplex emission (XplxE) generated by re-combined RIP could be influenced by an external magnetic field. Interconversion between electronic spin states in RIP under the magnetic field was described by the radical pair mechanism. In an optimized working solvent (anisole/DMF, v/v=50/50) and 375-nm illumination, its exciplex emission with an external magnetic field (>50 mT) becomes 1.33 times brighter than that with zero field. The increased amount of emission is sufficient for imaging within a short time. An image of magnetic field distribution in microscale was obtained by epi-microscopy. Since 375-nm LED lamp illumination and short data acquisition time, our imaging microscope was free from photo-bleaching. Using 375-nm light source enable to build microscope composed of common and low-cost optical material with high transmittance in 375 nm. We also demonstrated its feasibility for a 3D-image of magnetic field with two-photon fluorescence microscopy.

Oral Presentation : **PHYS1.O-2**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:10

Chair: Ilsun Yoon (Chungnam National University)

Ultrafast Solvent-Coupled Charge Transfer in N-annulated Complex with Donor-Acceptor Conjugation

Changwon Kim, Tae Wu Kim¹, Chen Li², Hyotcherl Ihee*

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

¹*Chemical Sciences and Engineering, Argonne National Laboratory, United States*

²*Polymer Research, Max Planck Institute, Germany*

With the development of metal-free donor-acceptor dyes used in dye-sensitized solar cells (DSSCs), understanding the charge transfer character which plays a role in a prior step for electron injection to the electrode in DSSCs is important and the excited-state dynamics in donor-acceptor dyes are widely studied in many fields. Here, we explored the intramolecular charge transfer (ICT) dynamics in the excited state of the diphenylamine N-annulated naphthalene monoimide (DPA-N-NMI) dye, and found that its ICT dynamics shows dependence on the solvent polarity. We characterized its photophysical properties by steady-state absorption/emission spectroscopy and femtosecond broadband transient absorption (TA) spectroscopy, and observed that the transient spectra of the Franck-Condon (FC) state spectrally evolve to the those of the ICT state, which undergoes non-radiative relaxation with conformational rearrangement in polar solvents after photoexcitation. The transition from the FC state to the ICT state and the relaxation of the ICT state within ultrafast time regime are coupled to solvation dynamics, which were identified by extracting the solvation time correlation function. This correlation underlines that the ultrafast charge carrier dynamics is strongly affected by the solvation dynamics dependent on the solvent polarity. The understanding of the ICT dynamics unveiled in this study may offer the comprehensive insights for the carrier dynamics in DSSCs and can contribute to the effective design of dyes.

Oral Presentation : **PHYS1.O-3**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:20

Chair: Ilsun Yoon (Chungnam National University)

Twist-angle dependent optical second-harmonic generation from transition metal dichalcogenides (TMD) heterostructures

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. The SHG signal from artificially-stacked MoS₂ bilayers can be understood as a superposition of SHG fields from the individual layers. However, this model has not been verified for TMD heterostructures. Here, we studied the SHG behavior of TMD hetero-bilayers of varying twist angle in comparison with homo-bilayers. When homo-bilayers were rotated over 2π -azimuth with a fundamental beam normally incident on their basal planes, the polarization-resolved SHG signal exhibited a six-petal pattern with six azimuthal nodes, which agreed with the superposition model. The heterostructures, however, lacked the angular nodes because of an azimuth-independent signal in addition to the six-petal pattern. The fractional contribution of the constant signal was larger for more staggered hetero-bilayers. To explain these results, we propose that the anomaly originates from a non-zero phase difference between SHG fields generated in the individual monolayers. In addition, we show that the degree of the anomaly is sensitive to the fundamental's wavelength, as the phase depends on photon energy.

Oral Presentation : **PHYS1.O-4**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:30

Chair: Ilsun Yoon (Chungnam National University)

Highly efficient, mode-specific vibrational excitation of organic-molecules by plasmon-induced electrons

Hyun-Hang Shin, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

We observed abnormally intense anti-Stokes SERS peak of symmetric NO stretching (ν_{NO}) of 4-nitrobenzenethiol (NBT) molecules placed at plasmonic gaps. Corresponding effective vibrational temperatures are found to be 550 K. Such vibrational excitation occurs during the early stage of photo-reduction of NBT, whereas non-reactive aromatic thiols with similar structures (such as 4-mercaptobenzonitrile, 4-methylbenzenethiol) do not show any sign of vibrational excitation. This mode-specific excitation is successfully reproduced by inelastic resonant scattering of electrons ejected from the metallic surface. The chemical specificity of the events and local field dependence of anti-Stokes ν_{NO} intensity strongly support our modelling also. Furthermore, wavelength dependence of the anti-Stokes ν_{NO} intensity indicates that the electron originates from the excitation of localized surface plasmons of nanostructures.

Oral Presentation : **PHYS1.O-5**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:40

Chair: Ilsun Yoon (Chungnam National University)

Understanding gas behavior in local pores of Metal-Organic Frameworks by gas adsorption crystallography

Hae Sung Cho, Osamu Terasaki*

School of Physical Science and Technology, ShanghaiTech University, China

Gas adsorption is an essential and reliable characterization method for porous materials. Recently, we showed that in-situ X-ray scattering profiles along the complete pore filling led to the discovery of extra-adsorption domain and superlattice formation in mesoporous metal-organic frameworks (MOFs) with single pore type [1]. This method, termed here generally as “gas adsorption crystallography”, allowed for the access to knowledge such as the subtle changes in lattice constant, strain of the framework, quantitative and spatial distribution of gases, reflecting the gas behavior at any stage in the isotherm. Here, we demonstrate an extension of gas adsorption crystallography to porous crystals containing multiple types of pore and show how gas adsorption isotherms can be accurately decomposed into multiple sub-isotherms corresponding to each type of pore within a material. Specifically, two MOFs, PCN-224 and ZIF-412 containing two and three different types of pore, respectively, are used to generate isotherms of individual pores by combining gas adsorption measurements with in-situ X-ray diffraction. This isotherm decomposition approach reveals previously inaccessible information concerning gas uptake capacity, surface area, accessible pore volume of each individual pore, as well as the impact of pore geometry on the uptake and distribution of different adsorbates within the pores.[1] Cho, H. S. et al. Nature 527, 503 (2015).

Oral Presentation : **PHYS1.O-6**

Oral Presentation for Young Physical Chemists I

Room 305+306, THU 09:50

Chair: Ilsun Yoon (Chungnam National University)

Optically active vibrational sum-frequency generation spectroscopy of chiral molecule in isotropic liquid

Taegon Lee, Sanghee Nah, Jun-taek Oh¹, Hanju Rhee*

Seoul Center, Korea Basic Science Institute, Korea

¹*Korea Basic Science Institute, Korea*

Vibrational optical activity (VOA) has proven to be of use in determining absolute configuration of small organic chiral molecule and conformation of biomolecules such as protein and DNA. However, conventional VOA techniques such as vibrational circular dichroism (VCD) and Raman optical activity (ROA) often suffer from the weak signal and huge achiral background problems, which hinder an effective measurement of the chiral signal and thus have limited its wide application. Vibrational sum-frequency generation (VSFG) spectroscopy is a well-known technique that has been used to study vibrational structure and dynamics of molecules on the surface or at the interface, where centrosymmetry is broken. Recently, we developed a femtosecond chiral VSFG technique based on quasi-null achiral background-free measurement. Interestingly, it was shown that an optically active (OA) femtosecond VSFG signal can be generated from chiral molecules *in isotropic bulk liquid, not just at the glass/liquid interface*. By using a combination of femtosecond (spectrally broad) mid-IR and picosecond (spectrally narrow) visible laser beams, we could obtain the OA VSFG spectra of chiral limonene in the C-H stretching frequency region without any frequency scan. We also found that the stereo-specific vibrational structures of the enantiomers can be distinguished by circular and linear polarization intensity differences (CID and LID) under particular polarization controls. In this talk, the concept and experimental details of chiral SFG spectroscopy will be presented and which hyperpolarizability tensors are involved in our observables will be discussed. We anticipate that this femtosecond OA VSFG technique will be of use in further developing ultrafast time-resolved chiroptical spectroscopy and chiral vibrational microscopy.

Oral Presentation : **PHYS2.O-1**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:00

Chair: Ilsun Yoon (Chungnam National University)

Fe-oxide nanoparticles/SiO₂ as a regenerative organic dye adsorbent

Hyun Ook Seo^{*}, Young Dok Kim^{1,*}

Department of Chemical and Energy Engineering, Sangmyung University, Korea

¹Department of Chemistry, Sungkyunkwan University, Korea

Mesoporous SiO₂ particles containing Fe-oxide nanoparticles (~10 nm) were prepared by a temperature-regulated chemical vapor deposition and a post-annealing process. The performances of mesoporous SiO₂ with and without Fe-oxide nanoparticles towards methylene blue (MB) removal from solution (MB concentration of 5 mg/l) were examined at room temperature under dark conditions. When the Fe-oxide nanoparticles were loaded on SiO₂ adsorbents, the initial adsorption capability of the fresh SiO₂ particles can be maintained after the regeneration process (400 °C-thermal annealing for 3 hrs). The results of FT-IR analyses of used bare SiO₂ and Fe-oxide/SiO₂ adsorbents before and after the regeneration process revealed that Fe-oxide nanoparticles were able to catalyze the thermal degradation of adsorbed MB molecules regenerating adsorption sites. The initial adsorption efficiency of SiO₂ particles with Fe-oxide nanoparticles can be also fully recovered by a 100 °C-thermal annealing.

Oral Presentation : **PHYS2.O-2**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:10

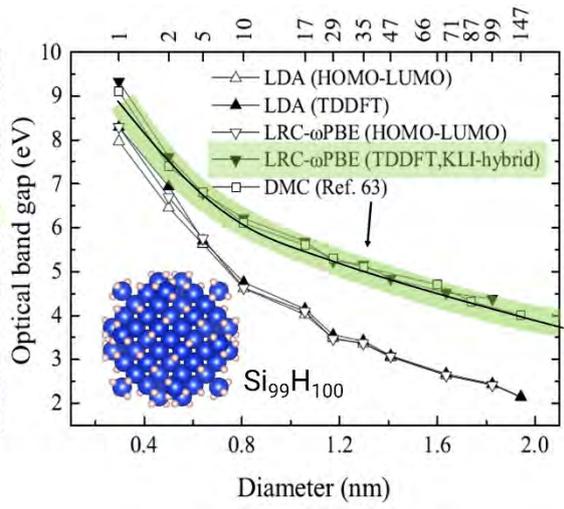
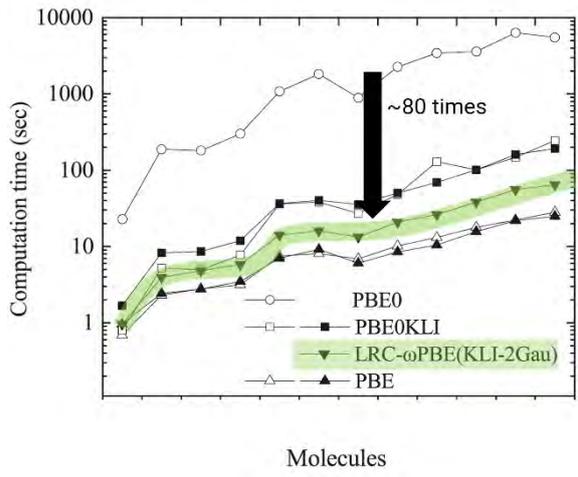
Chair: Ilsun Yoon (Chungnam National University)

Accelerating hybrid density functional calculation in real-space numerical grid methods

Jaewook Kim, Woo youn Kim*

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

Density functional theory (DFT) method attracts the chemist's attention nowadays, as the method can provide a reliable prediction of molecular properties or reaction mechanism with small computational costs. Especially, the emergence of the hybrid functional method makes the DFT calculation accurate enough to utilize to predict the chemical reaction mechanism. As the hybrid DFT calculation utilizes Hartree-Fock (HF) operator to get better energetics, efficient calculation of the HF exchange is essential to reduce computational cost. However, the HF calculation is computationally expensive in the case of the electronic structure calculation programs not adopting atomic-orbital based basis function, e.g., plane-wave basis set and real-space numerical grid method. In this presentation, I will introduce the ways to accelerate the computational speed of hybrid DFT calculation without sacrificing accuracy. First, the effect of the locality of the Kohn-Sham potential to the accuracy and efficiency of the hybrid DFT calculation will be discussed. Second, the adaptation of newly developed range-separated hybrid functional, LC-wPBE(2Gau), for the real-space based DFT program and its effect on the faster hybrid DFT calculation will be discussed.



Oral Presentation : **PHYS2.O-3**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:20

Chair: Ilsun Yoon (Chungnam National University)

Density Sensitivity Analysis of DFT: Measurement and Practical Solution

Suhwan Song, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

In present, many Density Functional Approximations (DFA) are developing and used by a bunch of science communities due to its practical yet accurate result compare to the ab-initio or experimental values. However, all exchange-correlation term inside the DFA is the approximation and, therefore, suffering from a certain amount of errors. In the case of electronic energies, such errors can be divided into two terms, Functional Error (FE) and the Density Driven Error (DDE) and they compete for each other to dominate the Total Error (TE). For past years, DDE dominant cases, so-called abnormal case, were successfully treated by the Density-Corrected Density Functional Theory (DC-DFT) scheme. But, it is very challenging for calculating the exact DDE due to its inherent usage of the exact electronical density. In this presentation, we will introduce a new concept, density sensitivity, and explains how to determine the degree of abnormality of a calculation in a given functional. By doing so, we can have the intuition whether the system needs to be treated by the DC-DFT scheme or just self-consistent DFT is good enough.

Oral Presentation : **PHYS2.O-4**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:30

Chair: Ilsun Yoon (Chungnam National University)

Eliminating spin-contamination of spin-flip time dependent density functional theory within linear response formalism by the use of zeroth-order mixed-reference (MR) reduced density matrix

Seunghoon Lee, Sangyoub Lee, Cheol Ho Choi^{1,*}

Division of Chemistry, Seoul National University, Korea

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

The use of mixed-reference (MR) reduced density matrix, which combines reduced density matrices of the $M_S = +1$ and -1 triplet-ground states, is proposed in the context of the collinear SF-TDDFT methodology. The time-dependent Kohn-Sham equation with the mixed state is solved by the use of spinor-like open-shell orbitals within the linear-response formalism, which enables to generate additional configurations in the realm of TDDFT. The resulting MRSF-TDDFT computational scheme has several advantages before the conventional collinear SF-TDDFT. The spin-contamination of the response states of SF-TDDFT is nearly removed. This considerably simplifies the identification of the excited states, especially in the "black-box" type applications, such as the automatic geometry optimization, reaction path following, or molecular dynamics simulations. With the new methodology, the accuracy of the description of the excited states is improved as compared to the collinear SF-TDDFT. Several examples, which include systems typified by strong non-dynamic correlation, orbital (near) degeneracy, conical intersections, and non-adiabatic dynamic simulation, are given to illustrate the performance of the new method.

Oral Presentation : **PHYS2.O-5**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:40

Chair: Ilsun Yoon (Chungnam National University)

Non-equilibrium Conformation of a Polymer Chain during Packaging and its Effect on the Packaging Rate

Seulki Kwon, Bong June Sung*

Department of Chemistry, Sogang University, Korea

The conformational relaxation of a polymer chain often slows down in biological and engineering processes. The polymer may stay in non-equilibrium states throughout the process such that one cannot invoke the local thermal equilibrium (LTE) approximation, which has been usually employed to describe various processes. In this letter, motivated by recent single-molecule experiments on DNA packaging into a viral capsid, we investigate how the non-equilibrium conformations would affect the packaging of a polymer chain into small confinement. We employ a simple but generic coarse-grained model and Langevin dynamics simulations to investigate the packaging kinetics. The polymer segments (both inside and outside the confinement) stay away from equilibrium under strong external force. By imposing the simulation condition to invoke the LTE, we find that the relaxation of non-equilibrium conformations plays a critical role in regulating the packaging rate.

Oral Presentation : **PHYS2.O-6**

Oral Presentation for Young Physical Chemists II

Room 305+306, THU 10:50

Chair: Ilsun Yoon (Chungnam National University)

Theoretical Studies on the Li-ion Conductivity of Solid-State Electrolytes: $\text{Li}_{6-x}\text{PS}_{5-x}\text{Cl}_{1+x}$

Byeongsun Jun, Sang Uck Lee*

Department of Bionano Engineering, Hanyang University, Korea

The safety issue of Li-ion battery (LIB) has been extremely emerged as the increase in size of LIBs for electrical cars and devices because of flammable organic electrolytes. After discovering Li superionic conductors, such as $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ (LGPS) and $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO), huge of researches have been promoted to replace organic electrolytes with nonflammable ceramic solid electrolytes. Argyrodites $\text{Li}_6\text{PS}_5\text{Cl}$ is also a candidate material for all-solid-state rechargeable LIBs with a high Li-ion conductivity of almost 0.1 to 1 mS/cm. However, it is necessary to improve the Li-ion conductivity of this material to use in commercial LIBs. In this work, we theoretically elucidated the Li-ion conductivity significantly increased as the amount of Li-ion is changed (both Li excess and shortage structures). We designed the crystal structures by controlling ratio x in $\text{Li}_{6-x}\text{S}_{5-x}\text{Cl}_{1+x}$. The calculated Li-ion conductivity at 300 K was 9.24 mS/cm, 0.02 mS/cm, 6.72 mS/cm and 35.01 mS/cm for $\text{Li}_{6.25}\text{PS}_{5.25}\text{Cl}_{0.75}$, $\text{Li}_6\text{PS}_5\text{Cl}$, $\text{Li}_{5.875}\text{PS}_{4.875}\text{Cl}_{1.125}$ and $\text{Li}_{5.75}\text{PS}_{4.75}\text{Cl}_{1.25}$, respectively. We expect the increased conductivity was originated from lowered energy barriers of the concerted Li-ion diffusion. Our results provide a possibility of improving alkali-ion conductivity of superionic conductors by controlling the amount of Li-ion in the crystal structures.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:00

Chair: Jae-Min Lim (Changwon National University)

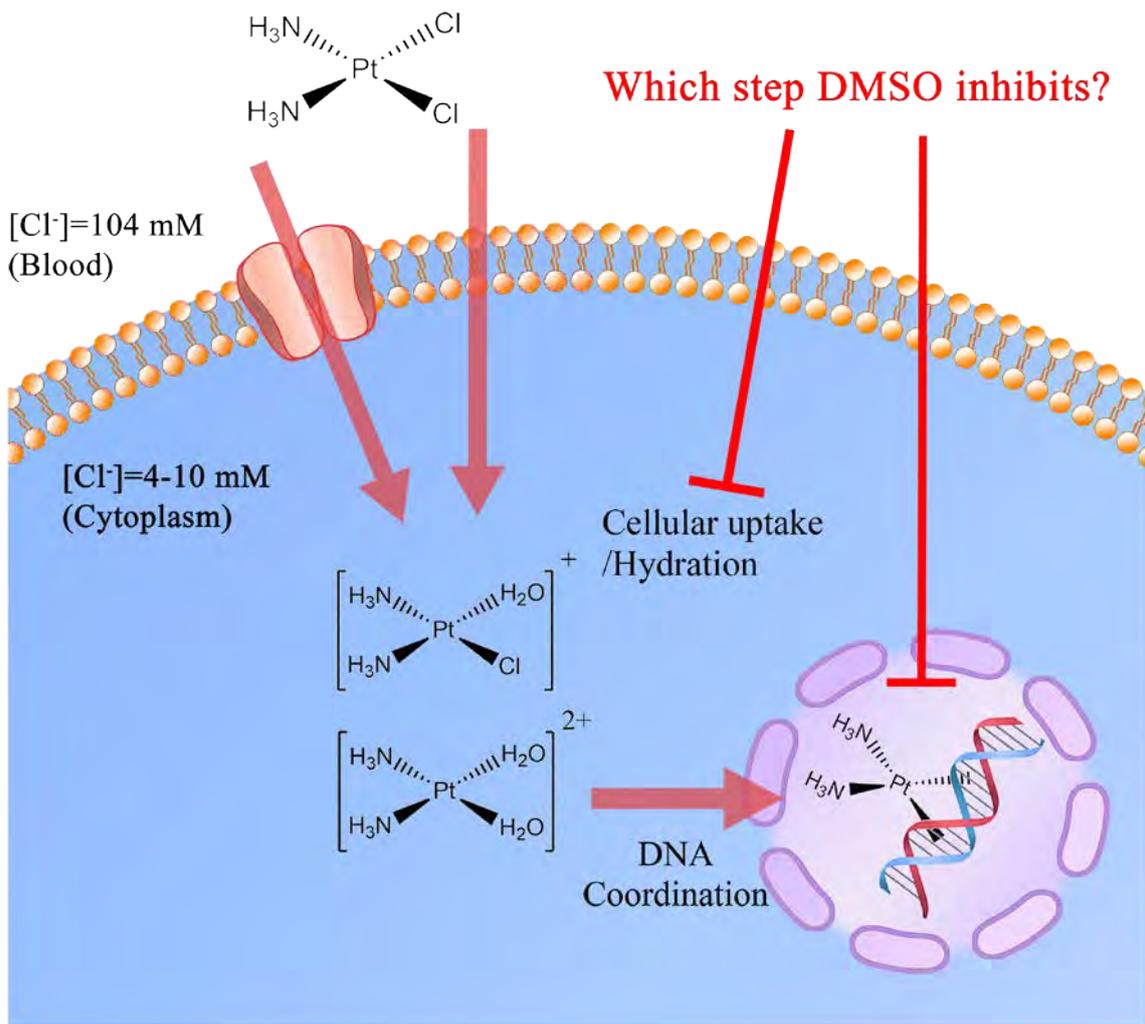
Investigating the deteriorated drug efficiency of cisplatin induced by DMSO using ICP-MS

Gyeongseo Min, Paul Valery Migisha Ntwali , Jong Yoon Han, Chae Eun Heo, Sooyeon Chae, Min Ji Kim, MyungKook Son, Chae Ri Park, Chaehyeon Yoon, Dongjoon Im, Hugh

I. Kim*

Department of Chemistry, Korea University, Korea

Cisplatin (cis-[Pt(NH₃)₂Cl₂]) is a platinum-based anticancer drug used for diverse cancers. Cisplatin is commonly administered as a single drug or in combination with other drugs to raise its efficacy. Nevertheless, cancer cells could have acquired or intrinsic resistance to cisplatin. For this reason, a large number of *in vitro* studies have been conducted to clarify the mechanism of this phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin and other drugs due to its ability to dissolve drugs in high concentration. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl⁻. However, it remains undefined that DMSO affects which specific step and deteriorates the efficacy of cisplatin *in vitro*. Herein, we employed an inductively coupled plasma mass spectrometry (ICP-MS) for the quantitative analysis of cisplatin to understand how DMSO directly impedes Pt-mediated toxicity. Our quantitative results show that taken amount of cisplatin is similar regardless of the solvents (i.e. media and 0.5% DMSO in media). However, DNA-Pt adduct formation, which is a direct cause of cell apoptosis, is significantly reduced for the cells treated with cisplatin dissolved in DMSO compared to those treated with cisplatin dissolved in media. ESI-MS results also show that the reduced DNA-Pt adduction is correlated to the exchange of cisplatin with DMSO. Overall, our study would provide valuable insight into the reduced efficacy of cisplatin for cancer treatment in the presence of DMSO, based on the correlation with structural change of cisplatin induced by DMSO.



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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:04

Chair: Jae-Min Lim (Changwon National University)

Prediction of chromatographic elution order of analytes from quantitative structure retention time relationship via quadratic programming

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Prediction of retention time from molecular structure using quantitative structure-retention relationships (QSRRs) is a powerful tool for method development in reversed-phase high performance liquid chromatography (RP-HPLC). Recently, retention order predicted from QSRRs is gaining increasing attentions when identifying peptides in shotgun proteomics. However, its fundamental limitation lies in the fact that low error in prediction of retention time does not necessarily guarantee that in prediction of retention order. This work reports prediction of retention order using QSRRs solved through quadratic programming (QP). A typical least squares problem was transformed into the standard QP formulation employing predicted retention times as inequality constraints. Two case studies: (i) separation of organic molecules on PLRP-S (PRP-1), 15.0 * 0.46 cm I. D., (Polymer Laboratories, Amherst, MA), made of cross-linked polystyrene (divinylbenzene) ($t_G = 20$ min, $T = 40$ °C); (ii) separation of on peptides silica gel Supelcosil-LC C18-DB, 15.0 * 0.46 cm I. D., ($t_G = 10$ min, $T = 35$ °C); on two columns are evaluated. Results have shown that when compared to control calculations in the first case study for PRP-1 columns, the average increase in retention time error, while the average decrease in retention order error. Results of the second case study for Supelcosil LC columns have shown the average slightly increased in retention time error, while the average decreased slightly in retention order error than in the first case study.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:08

Chair: Jae-Min Lim (Changwon National University)

Absolute Quantitation of Non-Human Glycan (Neu5Gc) in Human Biopsy Tissue by LC/MRM-MS

Nari Seo, Myung Jin Oh, Hyun Joo An*

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

N-Glycolylneuraminic acid (Neu5Gc), which cannot be synthesized in human, is an immunogenic sugar of dietary source. Neu5Gc in blood and tissue metabolically promote a variety of cell-to-cell adhesion processes in inflammation and the immune response related to cancer, cardiovascular, and inflammatory diseases. Thus, Neu5Gc in human has been considered as the indication of inflammation-mediated diseases, and their level has attracted more attention for monitoring disease progression and/or response to therapy. Although several Neu5Gc quantitation methods have been proposed for disease marker, determination of the levels of Neu5Gc in individual human samples is still challenging because there are very low amounts of Neu5Gc (less than 0.01% of the total sialic acids). Here, we have developed the MRM-based assay for the first time to quantify Neu5Gc from one shot biopsy gastric tissues, proved that the amount of Neu5Gc was correlated with cancer. Gastric biopsy tissues of cancer patient (n=10) and healthy control (n=10) were obtained from Seoul National University Bundang Hospital in Korea. Each tissue (2-3 mg wet wt.) was chemically treated. Liberated Neu5Ac and Neu5Gc were chromatographically separated, then monitored by LC/MRM-MS. The quantitative calibration curve of Neu5Gc was linear over the range of 1.5 fmol/L to 1.5 $\mu\text{mol/L}$ (10^3) and its correlation coefficient (r^2) was >0.999 . Neu5Gc was successfully quantified in all samples from gastric cancer patients and healthy controls, and the concentration of Neu5Gc was determined at fmol levels per one biopsy tissue. When compared to absolute abundances of Neu5Gc between controls and patients, expression levels in patient cohorts were 1.5 to 2-folds higher than those in the control group. These results could be supporting that the existence of Neu5Gc in human is linked to the disease. The developed strategies might be a new paradigm for a complement to glyco-based current cancer screening platform.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:12

Chair: Jae-Min Lim (Changwon National University)

Proteomics Approach for Plasma Exosomes in Lung Cancer Patients

**Jihoon Shin, Jinwook Lee, Min-gyu Youn, Miseon Jeong, Junghoon Kang, Wonryeon
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¹Department of Bio-nanochemistry, Wonkwang University, Korea

Exosomes are cell-derived nanovesicles that are rich source of novel biomarkers in the diagnosis and prognosis of disease. Exosomes have highly-specialized functions and play a key role in processing intercellular signaling. They are present in many complex biological fluids such as plasma. This study intends to identify exosome biomarker from lung cancer plasma. Exosomes were individually extracted from 46 patients' plasma of lung cancer through size-exclusion chromatography. Each exosome sample was pooled into three TNM groups. Each group of exosome samples from lung cancer patients was lysed with RIPA buffer. After Lysis, separated proteins from exosome were trypsin digested. Each group samples were identified nLC-MS/MS using Orbitrap Elite multiple times with various methods for exosomal protein identification from lung cancer plasma.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:16

Chair: Jae-Min Lim (Changwon National University)

A new approach for size determination of nanoparticles by single particle inductively coupled plasma-mass spectrometry (sp-ICP-MS)

Yeon Hee Park, Heung Bin Lim*

Department of Chemistry, Dankook University, Korea

A new approach for the size determination of Au nanoparticles in the size range of 15 nm – 100 nm was explored using single particle inductively coupled plasma-mass spectrometer (sp-ICP-MS). Since current sp-ICP-MS employed aqueous standard solutions to determine the particle size, many assumptions were made and experimental parameters should be determined, which caused measurement errors, although providing universality. In this work, several points were improved to enhance analytical performance in sp-ICP-MS. For higher sensitivity, the level of background subtraction was carefully determined after fitting to a normal distribution, followed by building a correlation curve of average intensity area per particle vs particle radius. When the results were fitted to an allometric function of $Y=aX^3$ at the optimized level of mean plus 3σ , excellent agreement was found, showing a correlation coefficient (R^2) of 0.995

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:20

Chair: Jae-Min Lim (Changwon National University)

A resistance study of serum-starvated neuroblastoma cell at specific drug concentration

Sooyeon Chae, Jong Yoon Han, Chae Eun Heo, Min Gyeongseo, MyungKook Son, Min Ji Kim, Hugh I. Kim, Chae Ri Park, Dongjoon Im, Chaehyeon Yoon, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is a solid tumor that arises from the developing sympathetic nervous system. As neuroblastoma belongs to heterogeneous disease, designing effective treatment for each patient is challenging. To examine individual variation in drug response, drug stability and efficiency tests are commonly performed in 2-dimensional (2D) cell or xenograft before clinical trial. However, additional condition to in vitro systems is crucial to closely mimic the complexity of in vivo system. Serum starvation is one of the most frequently used methods to imitate in vivo microenvironment. Thus, examining drug efficacy and resistance of serum-starved 2D cell has been suggested as a screening strategy for individual therapy. However, the differences between serum-starved and normal cells have not been fully understood. In this study, we studied the drug resistance in cancer cell depending on serum starvation. Especially, Topotecan, one of the anticancer drugs which inhibit DNA synthesis, was used. We observed that neuroblastoma cells in serum starvation show the resistance when they are treated with 1 μ M topotecan. Then, quantitation of drug uptake using reverse phase liquid chromatography-triple quadrupole mass spectrometry were performed. As a result of the quantitation of drug uptake, Serum starvation conditions showed relatively lower uptake at 48 hours when chemoresistance occurs. In correlation to distinct change in cellular uptake, we also performed the proteomic analysis to find differentiated protein group related to resistance in serum starvation. The fundamental understanding of anticancer drugs resistance on serum starvation can provide prediction of strategy for individual therapy.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:24

Chair: Jae-Min Lim (Changwon National University)

Single Bubble Microextraction Coupled with Capillary Electrophoresis

Xamyo Noulorsaytour, Doo Soo Chung^{1,*}

Chemistry, Seoul National University, Laos

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

Headspace (HS) extraction is a technique that have been developed for analysis volatile compounds. In conventional HS extraction, analytes evaporated from a donor phase (acidic) to the headspace and can be enriched to an acceptor phase (basic). The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus a small acceptor volume is preferred. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME) coupled with CE using a basic run buffer solution inside capillary as an acceptor phase. To reduce the headspace area, and increase enrichment factor enriched in more smaller headspace, here we present a new technique, single bubble microextraction (SBME) coupled with CE. It is a simple technique and easy to conduct HS extraction of a small volume sample for CE analysis. To reduce the headspace area, a small air bubble was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor vial. Then, SBME-CE was performed using the acceptor plug remained in the capillary. All steps of SBME-CE were carried out automatically using a commercial CE instrument without any modification.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:28

Chair: Jae-Min Lim (Changwon National University)

Charge effect of ATP on changing self-assembly mechanism of amyloidogenic proteins

Chae Eun Heo, Jong Yoon Han, Sooyeon Chae, Chae Ri Park, MyungKook Son, Min Ji Kim, Dongjoon Im, Paul Valery Migisha Ntwali , Gyeongseo Min, Chaehyeon Yoon, Hugh

I. Kim*

Department of Chemistry, Korea University, Korea

Amyloid fibrillation is a biological process by which amyloid disease-related protein molecules are self-assembled by hydrophobic interactions. In human body, such amyloidogenic proteins (e.g. amyloid- β , α -synuclein, human islet amylin polypeptide, tau, lysozyme and insulin) exist with specific charge state, positive or negative, depending on their inherent isoelectric point. To build a well-aligned fibril by assembling same charged proteins, it must overcome the electrostatic repulsion between the same charged residues. Thus, numerous research has been reported that charged species abundant in our body (e.g. metal ion, DNA, nucleic acid, heparin, glycosaminoglycans etc.) influence to the mechanism of amyloid fibrillation by electrostatic interaction. Here, we have studied to understand the molecular mechanism of protein fibrillation under ATP, which is a small biological polyanion and is present in high levels in cell. Firstly, we have conducted the thioflavin T(ThT) assay which monitors the formation of amyloid fibril. To identify and characterize the protein complexes between protein and small molecules, we have utilized electrospray ionization mass spectrometry (ESI-MS) and ion mobility spectrometry (IMS), along with circular dichroism (CD) and solution small-angle x-ray scattering (SAXS). The experimental evidence obtained from these diverse analytical techniques, and subsequent studies about biological anion-mediated protein aggregation would be highly helpful in understanding the mechanistic details of amyloid fibrillation under the influence of external factors, which affect protein-protein interactions.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:32

Chair: Jae-Min Lim (Changwon National University)

Profiling of lipoproteins from post-menopausal patients with osteoporosis by asymmetrical flow field-flow fractionation and nUHPLC-ESI-MS/MS

Kang Geun Lee, Joon Seon Yang¹, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

¹*The Resource Center for Stable Isotope-Resolved Metabolomics, University of Kentucky, United States*

Pathological mechanism of osteoporosis is not clearly known, but osteocytes affected by oxidized lipids are expected to be one of major factors. Bone mineral density (BMD) reaches the highest level in the age of 30s and decreases slowly over time, but symptoms are scarcely detected and it already gets serious when found out. Lipids play important roles in signal transduction, cell formation and various cellular processes. therefore, they are expected to be possible biomarkers to several diseases. Therefore, it is important to study relationships between lipids consisting lipoproteins in plasma and osteoporosis for early diagnosis. There are several studies about the relationship between lipids and osteoporosis in which BMD showed a meaningful correlation with low-density lipoprotein (LDL) and high-density lipoprotein (HDL). However, none of them conducted quantitative and qualitative analysis by using mass spectroscopy to differentiate lipid species at the molecular level in detail. In this study, 39 female plasma samples were classified into three groups : women having osteoporosis with no history of other diseases (n=10), women having osteoporosis with history (n=7), and age-matched control (n=22). Flow field-flow fractionation (FIFFF) is a technique that can separate particles or macromolecules by size. Lipoproteins of blood samples were fractionated by sizes using asymmetrical flow field-flow fractionation and the lipids were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Overall, 341 lipids from patient's plasma were identified and 289 lipids were quantified with statistical evaluations for the screening species with significant alterations when osteoporosis was developed.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:36

Chair: Jae-Min Lim (Changwon National University)

Chemiluminescent probes-based paper strips for detection of influenza

Jinsol Han, Sharipov Mirkomil¹, Yong-ill Lee^{1,*}

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¹Department of Chemistry, Changwon National University, Korea

According to the World Health organization (WHO), millions of people are infected by influenza virus each year. Traditional diagnosis methods require high cost equipment and technician for diagnosis of influenza virus. Last decade, the development of alternative diagnosis techniques for influenza has received a tremendous attention of scientist. The emerging paper-based analytical devices (μ PAD) has shown their potential as low cost and easy to use method in 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 fluorescent probe or chemiluminescent is promising in development of novel, low-cost and easy to operate sensing material. 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 chemiluminescent derivative-based μ PAD that is selectively activated in the presence of influenza virus. μ PAD was designed via stacked system to ensure to deliver the influenza virus to the target area after deposition onto μ PAD.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:40

Chair: Jae-Min Lim (Changwon National University)

Oligomerization of tau protein mediated by electrostatic interaction with ATP

Jong yoon Han, Chae Eun Heo, MyungKook Son, Dongjoon Im, Gyeongseo Min, Sooyeon Chae, Chae Ri Park, Min Ji Kim, Paul Valery Migisha Ntwali , Hugh I. Kim*

Department of Chemistry, Korea University, Korea

The fibrillation of tau, a microtubule-binding protein, in neuron is a hallmark of Alzheimer's Disease. Although the detailed fibrillation mechanism of tau is not revealed, negatively charged biomolecules are considered as crucial factors which can induce tau fibrillation. Adenosine triphosphate (ATP) is an abundant anionic biomolecule with high charge density (1-10 mM in cytosol) and was recently suggested as a potential cause of tau fibrillation. In this study, we investigated the influence of ATP on the structural transition of tau K18 (a four-repeat domain crucial for tau fibrillation) using ion mobility mass spectrometry (IM-MS) and small angle x-ray scattering (SAXS). Our results imply that the ATP induces monomeric K18 to form dimers with the formation of partially folded structure. Overall, our study would be valuable for characterizing the role of ATP as a promoter to induce tau oligomerization in the early stage of fibrillation.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:44

Chair: Jae-Min Lim (Changwon National University)

Automated cold volume calibration of temperature variation in cryogenic hydrogen isotope sorption isotherm

Jaewoo Park, Minji Jung, Hyunchul Oh^{1,*}

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The gas adsorption isotherm requires accurate measurement for the analysis of porous materials which is used as an index of surface area, pore distribution, adsorption amount of gas. Basically, adsorption isotherms of porous materials were measured conventionally at 77K and 87K using liquid nitrogen and liquid argon. The cold volume calibration in such conventional way was simply done by splitting into two zone (cold and warm volume) through controlling level sensor in Dewar filled with liquid nitrogen or argon. As a result, the BET measurement for textural properties is mainly limited to the N₂ or Ar gas. In order to investigate the other gases at various temperature independently, a novel temperature control system for sample cell is required, and consequently the cold volume calibration at various temperature become more important. In this study, the cryocooler system is newly installed in commercial BET device for controlling the sample cell temperature, the automated cold volume calibration of temperature variation for various gases (e.g. hydrogen isotopes) is introduced. This developed calibration method presents reliability and reproducibility of the cryogenic measurements of hydrogen isotope separation in porous materials, and also provide the large flexibility for performing various other gases with temperature.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:48

Chair: Jae-Min Lim (Changwon National University)

Investigation of changes in serum lipid levels upon the partial hepatectomy of swine in relation to the post-hepatectomy liver failure using nanoflow UHPLC-ESI-MS/MS

HaeA Kim, JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Post-hepatectomy liver failure (PHLF) is the inability of the liver to perform its normal synthetic and metabolic function after liver resection to treat diseases like hepatocarcinoma. Despite much progress in hepatectomy, PHLF still has high morbidity and mortality. Therefore, PHLF is still a serious complication and a possible diagnostic method in its early development stage after surgery is required to be developed. In this experiment, the changes in serum lipid levels of swine serum were investigated according to the degree of liver resection and elapsed periods after operation using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS). Serum samples were collected at four time intervals: before the operation, after 14 hours, 30 hours, and 48 hours of partial hepatectomy operation from six sham swine which did an only laparotomy, seven swines with 70% partial hepatectomy (70% PHx), and seven PHLF swines (90% PHx) which underwent 90% partial hepatectomy. A total of 151 phospholipids, 22 sphingolipids, and 204 glycerolipids were structurally identified based on collision-induced dissociation (CID) experiments and each lipids species of individual serum sample was quantitatively analyzed using selective reaction monitoring (SRM) mode. The alterations in lipid levels between 70% PHx group and 90% PHx groups were statistically evaluated to discover candidate marker species showing significant differences.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:52

Chair: Jae-Min Lim (Changwon National University)

Optimization of nanoflow ultrahigh performance liquid chromatography (nUHPLC) conditions for high-throughput and rapid lipid analysis by ESI-MS/MS

Gwang Bin Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Since separation in the nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS) is carried out at nanoflow rate regimes, performances of separation can be improved with the increased resolution with the minimization of sample amounts to be injected and the consumption of organic solvents. However, when a large number of sample analysis is required, a high speed separation is necessary for nUHPLC compared to the typical gradient elution condition that requires 30 min for a separation of lipids with broad classes without incurring spectral congestion in MS detection. This study demonstrated that high-throughput and rapid lipid analysis can be carried out within 10 minutes of separation by adjusting gradient elution condition with the increase of flowrates but without increasing the spectral congestion. The average peak width can be decreased to 0.14 min for PC 16:0/16:0 in a 10 min run condition compared to 0.15 min for a 30 min run condition with the standard deviation of retention time in repeated measurements as 1.68 s. The plate numbers of PC 16:0/16:0 can be above 330,000. In addition, MS detection efficiencies of lipid species upon increasing separation speed was evaluated with lipid standards spiked to a serum sample.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 09:56

Chair: Jae-Min Lim (Changwon National University)

Effect of aging on lipidomic changes in mouse serum, kidney, and heart

Jung Yong Eum, JongCheol Lee¹, Myeong Hee Moon^{1,*}

Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Aging is defined as the gradual decline of metabolic functions and is becoming the global burden due to the extended human life expectancy. The detailed metabolism of aging is still not fully understood, but it is well known that aging causes intracellular accumulation of reactive oxygen species which could develop age-related diseases such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Since changes in lipid metabolism may induce these diseases, examining the alteration of lipid levels is important. In this study, using serum, kidney, and heart from the 4- and 25-month-old C57BL6 female mice, a comprehensive lipidomic analysis was done to elucidate age-induced perturbation of lipid profiles by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Among 542 identified lipid species, 279 lipid species were quantified in selected reaction monitoring mode. While most of the lipid species with significant changes (> 2 -fold, $p < 0.01$) were found to be decreased by aging, triacylglycerols were increased in mitochondria rich tissues, especially in the heart. The ratio of phosphatidylcholine over phosphatidylethanolamine (PC/PE) which was the important factor of mitochondria membrane integrity was found to be significantly decreased only in kidney. This presentation demonstrates that nUHPLC-ESI-MS/MS analysis can determine the lipid species showing significant changes in serum, kidney, and heart of aged mice.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:00

Chair: Jae-Min Lim (Changwon National University)

A study on the determination of inorganic arsenic by solid phase extraction and fs LA-ICP-MS

Seon Hwa Lee, Sang-Ho Nam*

Department of Chemistry, Mokpo National University, Korea

The toxicity of arsenic depend on the concentration and chemical structure present in the natural environment. Thus, the accurate determination of inorganic arsenic in various samples is necessary. IC-ICP-MS (Ion Chromatography-Inductively Coupled Plasma-Mass Spectrometry) is the most popular method for quantitative and qualitative determination of arsenic. However, the method has disadvantage of complex instrument, elaborate sample preparation and long analysis time. In this study, inorganic arsenic species were separated using a membrane filter disk with strong anion exchange in the SPE (Solid Phase Extraction) method, then determined by fs LA-ICP-MS (femtosecond Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry). The detection limit of inorganic arsenic was 0.095 $\mu\text{g}/\text{kg}$ by fs 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 from organic arsenics. The linear dynamic range was from 1 to 1000 $\mu\text{g}/\text{kg}$ by LA-ICP-MS, and the correlation coefficient was 0.99997. The recovery rate of the sample is close to 110%. A new method using solid phase extraction and fs LA-ICP-MS was the accurate and sensitive method for quantitative analysis of inorganic arsenic in a sample.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:04

Chair: Jae-Min Lim (Changwon National University)

Picogram detection of nitro-explosive compound using multiple emitting Polythiophenes-Coated CdTe QDs

Mohamed Ragab Elsayed Ali, Salah Mahmoud Tawfik Ahmed¹, Yong-ill Lee^{1,*}

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A facile in-situ polymerization strategy has been performed to synthesize novel multiple emitting amphiphilic conjugated polythiophene-coated CdTe quantum dots as an optical sensor for the rapid, sensitive, selective, and on-site detection of 2,4,6-trinitrophenol (TNP). More importantly, portable, disposable, cost-effective, and easy-to-use paper strips and chitosan film were successfully applied to visually detect TNP concentrations as low as 1 nM. Using a smartphone with an easy-to-access and color-scanning App as a detection platform for the quantitative determination of TNP has also been demonstrated. The quantum dot-based sensor not only exhibits an excellent selectivity for TNP comparing with its analogues, but also possesses an excellent limit of detection of 0.56 nmol L⁻¹ with linear ranges of 0.05-14 μmol L⁻¹. Furthermore, the quantum dot 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 1.54-2.32% and 1.44-2.81%, respectively. This work unveiled an effective method for the sensitive and selective detection of TNP explosive toward national security and environmental protection. **Keywords:** QDs, trinitrophenol (TNP), river water, electron transfer mechanism.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:08

Chair: Jae-Min Lim (Changwon National University)

Graphene oxide as a peroxidase mimetic catalyst for detection of Cr(VI) ions

Nguyen Ngoc Nghia, Huy B.t.¹, Yong-ill Lee^{1,*}

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Graphene oxide (GO) was used as a peroxidase mimetic catalyst to detect hexavalent chromium (Cr(VI)) in aqueous solutions. The color change of tetramethyl benzidine (TMB) which was catalyzed by GO. The color of the probe will be turned "OFF" and "ON" by adding 8-hydroxyquinoline (8-HQ) and Cr(VI), respectively. The mechanism could be explained due to the chelation reaction between 8-HQ and Cr(VI). The color change can be observed by naked eyes or UV-vis spectrophotometer. Under the optimal experimental conditions, the prepared probe exhibited high selectivity, limit of detection (6 nM), and large linear range. This study was applied successfully for Cr(VI) detection in real water. Keywords: hexavalent chromium; chelate; graphene oxide; mimetic catalyst; naked eyes.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:12

Chair: Jae-Min Lim (Changwon National University)

Nonionic alginate-coated upconversion nanoparticles functionalized with folic acid for selective NIR-imaging and pH-responsive drug delivery

Sharipov Mirkomil, Salah Mahmoud Tawfik Ahmed, Huy B.t., Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

Rare-earth upconversion nanoparticles (UCNPs) have been proposed as biological luminescent labels for the bioimaging application of future because of their property to convert NIR irradiation to visible light. However, their toxicity, low dispersion, and low selectivity call into question their suitability in nanomedicine. To address these challenges, naturally modified nonionic alginate-based polymers were successfully synthesized and coated onto upconversion nanoparticles (UCNPs) to act as functionalizing agents. The developed hybrid polymer-UCNPs nanoparticles have showed a high stability and excellent biocompatibility. These hybrid nanoparticles have shown a selective NIR imaging of KB cells due to the presence of folic acid. Moreover, the presence of large cavities of materials and amphiphilic polymer shell, these hybrid nanoparticles were able to efficiently load the anticancer drug doxorubicin (DOX) as well as to release it in highly controlled and selective manner via folate receptor-mediated endocytosis. Cytotoxicity test against KB cells have confirmed that hybrid nanoparticles loaded with DOX have a higher inhibition of growth of KB cells compared to free DOX. The developed theranostics platform is capable to simultaneously perform imaging and deliver anticancer drugs and thereby is expected to grant a valuable innovation in bioimaging and nanomedicinal applications.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:16

Chair: Jae-Min Lim (Changwon National University)

Gold nanostar-based SERS substrate for pesticide analysis

Hung Thai viet, Huy B.t.¹, Yong-ill Lee^{1,*}

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Pesticide has caused serious health implications to people and the environment even with a small amount. Surface-enhanced Raman scattering of gold and silver nanoparticle was a powerful analytical tool for the sensing of trace molecules. We synthesized gold nanostar by one step seedless method at room temperature. This method is easy, time- and energy-saving method and generated a rough and clean gold surface. Gold nanostars display tunable optical properties in the visible and near-infrared region which lead to a strong electromagnetic field enhancement. This has been applied to analyze trace pesticide at a small scale with high sensitivity and selectivity

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:20

Chair: Jae-Min Lim (Changwon National University)

Novel zwitterionic fluorescent polythiophene sensor for E.coli. detection

Jimin Shim, Salah Mahmoud Tawfik Ahmed, Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

We developed a novel zwitterionic fluorescent polythiophene with high sensitivity for the detection of gram-negative pathogenic bacteria. The sensing probe using the zwitterionic fluorescent polymer was constructed with three different water soluble thiophene monomers via oxidative polymerization reaction. The zwitterionic fluorescent polythiophene bound to bacteria through ionic complexes between anionic groups on the bacterial surface and cationic groups after 15 min incubation. This finding demonstrated that the fluorescence on system operated via changes in the hydrophilic and hydrophobic nature of the zwitterionic fluorescent polymer at pH (7.4), at a fixed polymer concentration. The limit of detection for *Escherichia coli* was found to be 0.033 cfu/mL with linear range from 1.15×10^8 - 1.15×10^9 cfu/mL. With these encouraging results, it is expected that it would open revenues for promising applications of zwitterionic polythiophene in real samples. **Keywords** : zwitterionic polythiophene, Gram-negative bacteria, E.coli, Fluorescence enhancement, Bacterial surface

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:24

Chair: Jae-Min Lim (Changwon National University)

Detection of C₁₈-ceramide through a novel μ PAD coupled with mass spectrometry

Shavkatjon Azizov, Sharipov Mirkomil, Salah Mahmoud Tawfik Ahmed, Huy B.t., Huy B.t., Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

We developed an innovative wax-printed microfluidic paper-based analytical device (μ PAD) coated with paraffin has been as a highly efficient and low-cost microfluidic device resistant to common mass spectrometry organic solvents. The prepared novel μ PAD-MS system has been introduced for the analysis of C₁₈-ceramide through complexation with metal ions. In contrast to simple paper spray system, the developed μ PAD has allowed the analysis of low concentration of C₁₈-ceramide due to the maximum supply of deposited analyte through a microchannel. The MS results established the formation of doubly and singly charged metal ion complexes between ceramide and different metal ions. Especially, the complexation that occurs between lithium ions and C₁₈-ceramide showed a high relative abundance over other formed complexes. The established μ PAD has shown its prospective in the analysis of hydrophobic biomolecules dissolved in organic solvents and at the same time to avoid their penetration through the developed barriers. The developed μ PAD-MS technique provides clear advantages over the other methods by reducing the number of experimental steps and simplifying the operation process for the identification of C₁₈-ceramide.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:28

Chair: Jae-Min Lim (Changwon National University)

Development of Novel Upconversion Nanoparticles Functionalized with Amphiphilic Polymers for detection of Alprenolol

Seung Ha Lee, Salah Mahmoud Tawfik Ahmed, Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

Upconversion nanoparticles (UCNPs) are a unique type of photoluminescence(PL) material in which lower energy excitation is converted into higher-energy emission via multi-photon absorption processes. In this research, novel amphiphilic copolymers were synthesized to act as functionalizing agents for NaLuGdF₄:Yb³⁺/Er³⁺ UCNPs. The UCNPs coated with amphiphilic copolymers were characterized by using FTIR, ¹HNMR, SEM, TEM, UV, and PL instruments. These materials were used as optical sensors to detect Alprenolol which is kind of high blood pressure treatment. Our developed sensors displayed good analytical performance such as low limits of detection and good linearity. Furthermore, the sensors were applied to determine the level of high blood pressure drugs in human urine and serum samples with good recoveries. **Keywords:** Upconversion nanoparticles, amphiphilic copolymers, optical sensors, alprenolol, human serum samples, human urine samples

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:32

Chair: Jae-Min Lim (Changwon National University)

Development of melamine specific bioreceptor using phage-display and their verification

ChanYeong Park, Seung Hoon Back, Tae Jung Park*

Department of Chemistry, Chung-Ang University, Korea

Recently, concerns about safety in food have increased, because carcinogens or illegal hazardous substance are discovered to cheat its component contents. There are many kinds of dangerous reagents, we have investigated the melamine. Originally, it was mostly employed to synthesize melamine-formaldehyde resins, laminates, and plastics. However, some people added the melamine in dairy products. Since the quality evaluation of dairy products is conducted by measuring nitrogen contents. The ingested melamine can crystallize in human renal and induce acute nephrolithiasis and kidney injury. Thus, the detection of melamine is the momentous issue. To detect the melamine, advanced analytical equipment such as liquid and gas chromatography, and Raman spectroscopy were introduced, but they demand for the skilled person, high cost, and long time. Even though the optical detection methods, such as colorimetry and fluorescence, are also being developed as another detection method, it is difficult to specifically detect the melamine since they just recognize the structural features of melamine like aromatic ring or hydrogen bond. In this regard, we have developed specific bioreceptors that selectively bind to the melamine through the phage-display technology. The technique has been used to find out the new bio-receptors for the target such as cell-surface proteins, chemical hapten, etc. In this study, we have discovered melamine-specific binding peptides and evaluated their specificity and affinity against the melamine using graphene oxide quantum dot (GOQD)-Hg²⁺ quenching system. As a result, they showed the high attraction for melamine with a low level of detection limit and appear the probability as a detection sensor for the electrochemical and colorimetric analyses.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:36

Chair: Jae-Min Lim (Changwon National University)

Mechanism of trinitrophenol explosive detection with novel multiple emitting quantum dots coated with amphiphilic conjugated polythiophenes

Sarvar Kakhkhorov, Salah Mahmoud Tawfik Ahmed¹, Yong-ill Lee^{1,*}

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The novel type of multiple emitting CdTe quantum dots (QDs) coated with amphiphilic conjugated polythiophenes has been developed for the determination of the 2,4,6-trinitrophenol (TNP) explosive. Overall, four types of nanohybrids were designed based on the QDs coated with differently charged polythiophenes (cationic, anionic, and nonionic) and thiophene copolymer. The integration of QDs aimed to increase the electron density of polythiophenes which resulted in efficient interaction of the developed nanohybrids with electron-deficient TNP. This was confirmed by considerable fluorescence quenching of the developed sensors when their response to various types of nitroexplosives was studied: nitrophenols and specifically TNP caused the most remarkable fluorescence quenching compared to the other nitroaromatics. Among the developed nanohybrids, positively charged polythiophenes demonstrated the most efficient fluorescence quenching due to the attraction of –OH groups of TNP to the surface of such nanohybrids. The results of time-resolved fluorescence measurements revealed the presence of static quenching through the formation of ground state electrostatic interactions which excludes the excited state energy transfer with Förster resonance energy transfer (FRET) mechanism and suggests the inner filter effect (IFE) as a reason of fluorescence quenching of the sensors. In addition, the contribution of hydrogen bonding, electrostatic, and π - π interactions formed between TNP and QD nanohybrids resulted in high fluorescence quenching of up to 96% as well as in the detection of ultralow amounts of TNP up to 0.56×10^{-9} M.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:40

Chair: Jae-Min Lim (Changwon National University)

Highly sensitive fluorescent sensor based on novel coordinated amphiphilic polythiophene nanohybrids for triacetone triperoxide explosive detection

Salah Mahmoud Tawfik Ahmed, Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

Triacetone triperoxide (TATP), one of the most dangerous primary explosives, has emerged as an explosive of choice for terrorists in recent years. A new strategy for the detection of TATP is developed by utilizing amphiphilic polythiophene-coated CdTe QDs (P1QDs) and Hg²⁺ ion. The emission of P1QDs is found to be quenched in the presence of Hg²⁺ ion by electron transfer. Upon addition of the TATP, the quencher (Hg²⁺ ion) has been removed from the surface of P1QDs owing to the strong interactions between TATP and metal ions (Hg²⁺ ion), which leads to significant fluorescence recovery of P1QDs. The detection limit for TATP is 87 µg/L. The simultaneous possession of high sensitivity and selectivity could enable this sensor to be potentially applicable for ultrasensitive and rapid detection trace of TATP in real samples. **Keywords:** amphiphilic polythiophene nanohybrids, metal ions, fluorescence recovery, triacetone triperoxide (TATP), real samples

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:44

Chair: Jae-Min Lim (Changwon National University)

Multi-element analysis of deciduous teeth by inductively coupled plasma mass spectrometry (ICP MS)

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Deciduous teeth have a unique characteristic that exposure chemicals accumulated at the prenatal period and at the postnatal period are spatially separated by the neonatal line in their microstructures. Because of this feature, deciduous teeth have been regarded as retrospective temporal biomarkers. In addition, deciduous teeth can provide direct signatures of fetal period exposures whereas other frequently-used biomarkers such as maternal blood, maternal urine, and cord blood can only give indirect ones. In the previous studies, we tried to develop a quantitative elemental analysis method for deciduous teeth by employing a microwave-assisted sample preparation method and inductively coupled plasma dynamic reaction cell mass spectrometry (ICP DRC MS). In this study, we validated a developed method with the bone meal standard reference material and applied a validated method to individual deciduous tooth samples. As a result, concentrations of over ten elements were successfully determined from five individual tooth samples and compared.

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

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:48

Chair: Jae-Min Lim (Changwon National University)

Optimization of sample preparation methods for the multi-class chemical analysis of the deciduous teeth

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Exposomics, a research field that tries to measure all the exposures of an individual and reveal how the measured exposures relate to health, receives an increasing attention. Recently, deciduous teeth have been proposed to be retrospective temporal biomarkers for exposomics researches due to its specific structure and growth pattern. However, sample preparation and analysis steps for the tooth matrix have not been explored extensively and need to be standardized. In this study, we evaluated various sample preparation procedures for extracting small organic chemicals from tooth samples and tried to develop a fast and reliable LC-MS/MS method for quantifying multi-class exposure chemicals. With the optimized sample preparation and analysis protocol, various environmental exposure chemicals such as phthalates, phenols, and paraben were quantitatively measured from the deciduous tooth samples.

Oral Presentation : **ANAL1.O-29**

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:52

Chair: Jae-Min Lim (Changwon National University)

High-throughput measurement of lipid turnover rates using 15T FT-ICR mass spectrometry

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Alteration in lipid dynamics is highly associated with various diseases including diabetes and atherosclerosis. Measuring *in vivo* lipid turnover rates at the molecular level can provide insight for better understanding of disease metabolism. The extensive occurrence of isomeric and isobaric lipids is a major bottleneck for studying lipid dynamics on a global scale by mass spectrometry (MS). An ultra-high resolution mass spectrometer is a promising solution to distinguish lipid isobars. In this presentation, we investigated the performance of Fourier Transform-Ion Cyclotron Resonance (FT-ICR) MS in the high-throughput measurement of lipid turnover rates in HeLa cell using partial deuterium oxide (D₂O) labeling. HeLa cells were cultured in 5% (mol/mol) D₂O enriched media and harvested at 8 different labeling times (0, 3, 6, 12, 18, 24, 36, and 48 hr). Lipid extracts from HeLa cell were separated by Ultra-Performance liquid chromatography and analyzed by ultra-high resolution 15T FT-ICR mass spectrometer for differentiation of lipid isobars. High-throughput determination of lipid turnover rates was performed on a global scale by employing our in-house built software. As a result, 424 and 192 lipids were identified at the species level in positive and negative ion mode, respectively. Turnover rates of 48 lipids covering 12 lipid subclasses were obtained in the range 0.0048 to 0.15 hr⁻¹.

Oral Presentation : **ANAL1.O-30**

Oral Presentation of Young Analytical Chemists I

Room 202, THU 10:56

Chair: Jae-Min Lim (Changwon National University)

Measurement of conversion yield of 7-dehydrocholesterol to previtamin D using liquid chromatography-mass spectrometry

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Korea*

Vitamin D is involved in many diseases including sleep disorders, bone metabolism, diabetes, and multiple sclerosis. It is formed from 7-dehydrocholesterol (7-DHC) present in the human skin. When 7-DHC receives UV-B (280-315 nm), it becomes previtamin D and then is converted to vitamin D by thermal isomerization. Herein, we report an analytical method to quantify the conversion yield of vitamin D from 7-DHC by UV irradiation based on liquid chromatography-mass spectrometry (LC-MS), which has a higher selectivity compared with conventional LC-UV. In order to find optimal irradiation conditions, the conversion yields of 7-DHC to previtamin D were measured by varying irradiation time and light source wavelength. After 7-DHC was exposed to a UV-B source in vitro with light intensity of 0.5 mW / cm² for 0-120 sec, 7-DHC, previtamin D, and vitamin D were separated on a Zorbax SB phenyl column and analyzed by a quadrupole-time-of-flight mass analyzer. The conversion yield of 7-DHC to previtamin D increased steadily with increasing irradiation time at all UV-B wavelengths and showed the maximum yield of 10% with UV-B irradiation for 120 sec at 285 nm.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:00

Chair: Jongwoo Lim (Seoul National University)

Electrochemical Immunosensor using Nanotriplex of Graphene Quantum Dots, Fe₃O₄, and Ag Nanoparticles for Tuberculosis

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Nano Fusion Technology, Ph.D. student at Pusan National University, Ethiopia

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Electrochemical technique is one of the powerful tools for characterization of NPs. The techniques have the potential to achieve rapid, sensitive, selective, and low-cost detection of biomolecules relevant to disease detection and diagnosis. Here, an electrochemical biosensor was developed for detection of mycobacterium tuberculosis (Mtb) antigen (CFP-10) using Fe₃O₄@Ag/GQD modified glassy carbon electrode (GCE) as a sensing platform and gold nanoparticles (AuNPs) as a label for signal amplification. The sensing platform was newly designed to obtain synergetic performance using three different nanomaterials; i.e., Fe₃O₄ for the purpose of increasing surface to volume ratio that strongly adsorb chemicals and rapidly transfer electrons, Ag for enhancing electrical conductivity to facilitate transfer of electrons and GQD increases surface area for capturing numerous primary antibodies (Ab1). A sandwich type immunoassay was prepared by immobilizing antibody 1 (Ab1), and AuNPs functionalized with antibody 2 (Ab2–AuNPs) on Fe₃O₄@Ag/GQD modified GCE. The immunosensor showed a wide linear range (0.005 - 500 µg/mL) with a limit of detection (LOD, S/N = 3) reaching 0.33 ng/mL. The result showed good performance with a high selectivity, and simple operation, can be easily extended to other pathogenic bacteria detection.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:04

Chair: Jongwoo Lim (Seoul National University)

Optical analysis of degree of deacetylation in chitosan

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Chitosan is one of promising polymers for applications in various fields. However, despite diverse research studies conducted on its biocompatibility, its uses are still limited. The main factor that can affect its physical, chemical and biological properties is the degree of deacetylation (DOD), which represents the proportion of deacetylated units in the polymer. In this article, the in vivo biocompatibility of chitosan-hydroxyapatite composite films composed of chitosan with different DOD values was investigated by traditional biological protocols and novel optical spectroscopic analyses. The DOD of the chitosan was estimated and calculated by Raman spectroscopy, Fourier transform infrared spectroscopy, and proton nuclear magnetic resonance spectroscopy. The chitosan with the higher DOD induced a higher incidence of inflammation in skin cells. The amino group density, biodegradability, and crystallinity of chitosan are three possible factors that need to be considered when determining the biocompatibility of the films for in vivo application, since they led to complicated biological results, resulting in either better or worse inflammation even when using chitosan products with the same DOD. This basic study on the relationship between the DOD and inflammation is valuable for the development of further chitosan-based researches.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:08

Chair: Jongwoo Lim (Seoul National University)

Tuning plasmonic properties of 0-3D metastructure with self-assembled magnetoplasmonic nanoparticles

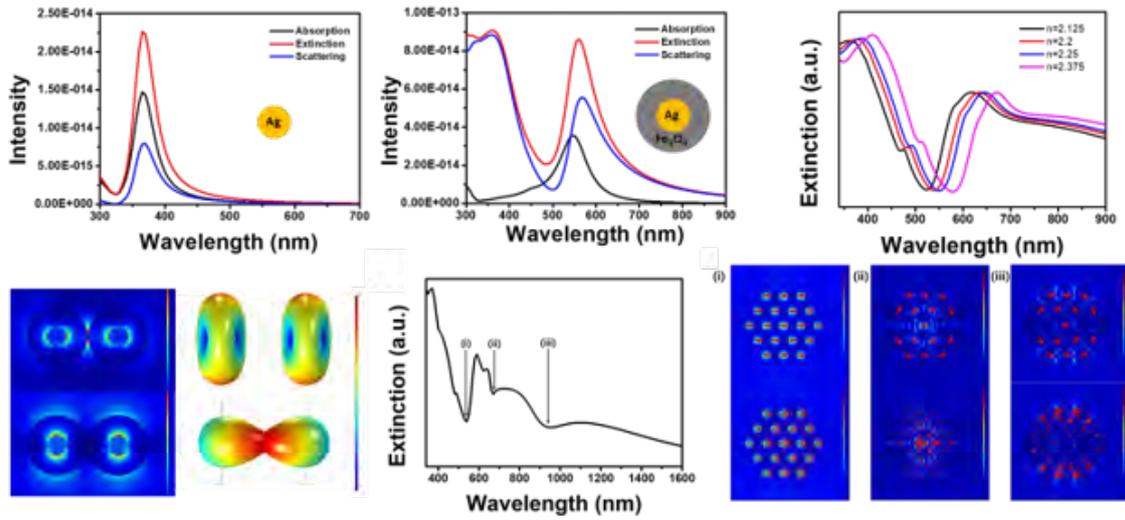
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Magneto-plasmonic nanostructures have been interested to the researchers in the fields such as optics, electronics and bio-engineering. They have been interested in its properties which can be explained with the concept of localized surface plasmon resonance. On the other side many researchers tried to fabricate metamaterials, the structure which shows abnormal optical property because of its permittivity and permeability which can be tuned by the periodic structures. We self-assembled nanoparticles into 1-3D suprastructure to make one kind of metamaterial. Moreover, we simulated absorption and scattering spectra of self-assembled suprastructure of Ag@Fe₃O₄ nanoparticles by using finite element method (FEM). We solved time-harmonic electromagnetic field distributions based on Maxwell's equation. We integrated energy loss on the surface and the volume of nanoparticles to plot extinction, scattering and absorption. Optical properties of single Ag@Fe₃O₄ nanoparticle in different condition was simulated. Moreover, 1-3D and chiral self-assembled structure of single nanoparticle was also simulated.



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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:12

Chair: Jongwoo Lim (Seoul National University)

An Synthetic Approach to Si/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 OH-doped graphene quantum dots (OH-GQDs) 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. For characterization FTIR, HR-XPS, XRD and electrochemical testing was performed. This nano-architecture significantly improved the structural stability and conductivity, which could be used as anode material for lithium secondary batteries.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:16

Chair: Jongwoo Lim (Seoul National University)

Characteristics and Electrochemical Performance of Graphene/Carbon nanofiber/Silicon Composites as Anode Material for Binder-Free Lithium Secondary Batteries

Ruye Cong, Jin-Yeong Choi, Chang-Seop Lee*

Department of Chemistry, Keimyung University, Korea

We report the interfacial study of a Graphene/Carbon nanofiber/Silicon Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon nanofibers (CNFs) were grown via chemical vapor deposition method with an iron-copper catalysts. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 700°C, and maintained for 30 min to synthesize CNFs. GO aqueous dispersion was added into the CNFs/Silicon solution, and the mixture was sonicated for 6h to obtain a GO/CNFs/Silicon aqueous dispersion. Electrode was fabricated by flow-directed vacuum filtration of GO/CNFs/Silicon aqueous dispersion through a filter membrane (90 mm in diameter and 0.22 μm in pore diameter) followed by air drying and peeling off from the filter. The morphologies, compositions and crystal quality of the prepared Graphene/CNFs/Silicon composites were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of Graphene/CNFs/Silicon composites as an anode of Li secondary batteries were investigated using three-electrode cell. The galvanostatic charge-discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:20

Chair: Jongwoo Lim (Seoul National University)

Synthesis, dispersion and tribological performance of alkyl functionalized graphene oxide and graphene-WS₂ Composites as an oil lubricant additive

Jong Seok Han, Jin-Yeong Choi, Chang-Seop Lee*

Department of Chemistry, Keimyung University, Korea

Graphene and WS₂ 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. GO is 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 First, We have painted a long alkyl chain of graphene oxide (GO) to improve the dispersion of oil-based lubricants with greatly enhanced lipophilicity. Second, a gelator is used for dispersion and a graphene-WS₂ composite is synthesized to improve lubrication performance. 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 (PAO oil) and oil containing WS₂ and also ultrasonicated for dispersion. Graphene-WS₂ composites were synthesized by hydrothermal synthesis, Graphene-WS₂ composites were added to the PAO oil with 1 wt% of the gelator. Chemical and structural properties of the synthesized alkyl functionalized graphene and Graphene-WS₂ composites 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.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:24

Chair: Jongwoo Lim (Seoul National University)

Combined Anion and Nonionic Surfactants-based Micellar Electrokinetic Chromatography with Laser-induced Fluorescence Detection for Quantification of Native Capsaicinoids

Yucheng Sun, Seong Ho Kang^{1,*}

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Micellar electrokinetic chromatography (MEKC) equipped with laser-induced fluorescence (LIF) detector was presented for highly sensitive detection of native capsaicinoids. Under running buffer condition of 450 nM Tween 20-15 mM sodium borate-2.2 mM SDS (pH 10), limits of detection (LODs) for capsaicin and dihydrocapsaicin reached 1.3 pM and 3.4 pM, respectively. However, the LODs in UV absorption detection for capsaicin and dihydrocapsaicin was 5.5 nM and 8.1 nM, respectively, demonstrating the presented modality was more sensitive for the capsaicinoids detection. Meanwhile, the mixed micellar surfactants, Twee20-SDS, contributed for improving the separation selectivity and efficiency. In addition, quantification of chili pepper, baechu and kimchi showed 98% confidence indicating there is no significant difference between MEKC-LIF and high-performance liquid chromatography (HPLC). The results demonstrated the developed MEKC-LIF method could provide sensitive on-line detection of capsaicinoids in various foods.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:28

Chair: Jongwoo Lim (Seoul National University)

Single-Molecule Nanocatalysis for Location Effect of Gold Nanoparticle on Carbon Nanotube

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Gold nanoparticles were immobilized on carbon nanotubes by two ways: filling of Au nanoparticles inside the CNT channels (Au/CNTs-in) by capillary action and dispersion of Au nanoparticles on the exterior surfaces of CNTs (Au/CNTs-out) by block the CNT channels. The locations of Au nanoparticles were confirmed by transmission electron microscopy (TEM). Ensemble catalytic activity measurements by UV-vis absorption spectrometer indicated that Au/CNTs-out had the higher catalytic activity than Au/CNTs-in. Single-molecule nanocatalysis experiments were carried out by lab-built prism-type total internal reflection fluorescence microscope (TIRFM) to reveal the location effect between Au/CNTs-in and Au/CNTs-out. The results indicated that Au/CNTs-out was more activity than Au/CNTs-in in reductive N-deoxygenation reaction of resazurin to resorufin. Furthermore, the product molecules on both Au/CNTs-out and Au/CNTs-in preferred the same pathway, reactant-assisted dissociation pathway, but different dissociation rates. The different catalytic performances of Au/CNTs-in and Au/CNTs-out were related to the electron density of Au nanoparticles caused by the its location and nature of CNTs.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:32

Chair: Jongwoo Lim (Seoul National University)

Feasibility of electrochemically modulated SERS measurement for improved differentiation of gallbladder diseases

Tung Vu, Eunjin Jang¹, Hoeil Chung*

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A screen-printed electrode (SPE) covered with three-dimensional gold nanodendrites (AuNDs) was used to measure SERS spectra of bile juices. To acquire SERS spectra with distinct features, a bile juice was pretreated with CH₃Cl-CH₃OH solution to eliminate hydrophobic components such as lipids and the remained aqueous hydrophilic phase was measured. Interestingly, Raman spectral features of the aqueous phase samples mostly resembled with those of bilirubin. So, it was presumed that the peaks were originated from conjugated-bilirubins, formed in a liver by attachment of sugars (such as glucuronic acid) to bilirubin (a heme break down product). Subsequently, conjugated-bilirubin becomes soluble in water. It expects that structure and composition of conjugated-bilirubin are dissimilar depends on different GB diseases (GB stone, polyp and cancer). Further, potentially improve the differentiation, varying electrochemical potentials were applied to the bile juice sample on SPE surface and corresponding SERS spectra were also acquired. Finally, principal component analysis (PCA) was used to qualitatively evaluate the degree of discrimination among these 3 GB diseases in the cases with and without application of electrochemical potential.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:36

Chair: Jongwoo Lim (Seoul National University)

Spatially offset based Raman scattering-based line-mapping as means to determine sample particle size

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Spatially offset based Raman scattering (SORS)-based line-mapping has been evaluated as a means for determining sample particle size. In SORS measurement, the position of Raman photon collection is away from that of laser excitation. As previously studied, the distribution of Raman photons became broader with the increase in particle size, as the mean free path of laser photons, the average photon travel distance between consecutive scattering locations, became longer under this situation. Therefore, when a SORS line mapping is performed along a packed powder sample, the peak intensities of sample in a series of the mapped spectra expect to decrease as offset distance becomes longer. Moreover, the slope in the change of intensity would be related with particle size, such as a greater slope for larger particle size. This possibility was the driving force for this research. For investigation, polyethylene (PE) powders with different particle sizes (300-200, 200-150, 150-100 and 100-75 micron) were prepared and SORS-line mapping was performed for each sample. Then, the slope of peak intensity was examined in relation with sample particle size. Various samples with different densities and refractive indices are under evaluation for deeper exploration.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:40

Chair: Jongwoo Lim (Seoul National University)

Infrared spectroscopic characterization of bile juices acquired from patients with gallbladder diseases

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Bile juice is a body fluid related with emulsifying and micellizing cholesterol in intestine, secreted in liver and stored in gallbladder (GB). Composition of bile juice would be different by health conditions of each patient; therefore, bile juice could be a beneficial medium for studying GB diseases. In this study, infrared (IR) spectroscopy has been used to study bile juices from patients of GB polyp and GB cancer. Before IR measurement, raw bile juice samples were pretreated with chloroform-methanol mixture solution to extract and separate organic, aqueous and protein agglomerates. Then, each phase-separated sample was dropped on hydrophobic OTS (octadecyltetrachlorosilane)-coated Si wafer to form reproducible circular droplet and dried for IR spectral acquisition. IR spectra were collected across a dried sample (line-mapping) and a representative spectrum was selected among the mapped spectra for further examination. In the chosen spectra, key spectral features related with GB polyp and GB cancer were searched and characterized. Next, to examine potential of IR spectroscopic discrimination of bile extracts according to diseases, principal component analysis (PCA) was used to reduce dimensions of spectral data into simply 2- or 3-dimensional score domains to easily recognize potential differences between GB polyp and cancer samples. In final, the future direction of this research will be discussed.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:44

Chair: Jongwoo Lim (Seoul National University)

Electrochemical study of fluorine doped lithium vanadium borate as a cathode material for lithium ion battery

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Recently, lithium transition metal borates, LiMBO_3 ($M = \text{Mn, Fe or Co}$), have been studied by many research groups due to low weight of $(\text{BO}_3)^{3-}$, relatively weak B-O bond, and high theoretical capacity. Its weaker B-O bond makes fast lithium ion diffusion. However, it has limitation because of their low ionic and electronic conductivities, which is revealed relatively low reversible capacity. Therefore, LiV_2BO_5 (LVBO) has been studied to improve operating potential, because multiple valence states of vanadium element can provide a high theoretical energy density. Also, fluorine doping in LVBO has been attempted to synthesis by sol-gel method. The morphology and composition of materials have been identified with scanning electron microscope and X-ray diffraction. The electrochemical properties are characterized by using galvanostatic charge/discharge and cyclic voltammetry measurements. The optimum doping ratio in LVBO is still under study with electrochemical properties.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:48

Chair: Jongwoo Lim (Seoul National University)

Various Multi-Facet Gold Bipyr amid Fabrication

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The seed-mediated growth of gold nanostructures has been shown to be strongly dependent on the gold seed nanocrystal structure. The gold seed solution can be prepared such that the seed are either single crystalline or multiply twinned. With added silver (I) in the cetyltrimethylammonium bromide (CTAB) aqueous growth solution, the two types of seeds yield either nanorods or elongated bipyr amidal nanoparticles. Or the combination of a Cl-containing surfactant with a low concentration of Ag plays a role in the stabilization of the {110} facets. In this study, we have investigated how different these solutions are and how controlled the aspect ratio of gold bipyr amid.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:52

Chair: Jongwoo Lim (Seoul National University)

Enhanced electrochemical performance of LiFeBO_3 cathode material via anion doped for lithium ion battery

Khoirul Umam, Youngil Lee*

Department of Chemistry, University of Ulsan, Indonesia

Anion-doped LiFeBO_3 cathode material has been successfully synthesized by solid-state method followed heat treatment. Fluorine was used as doping element to improve the conductivity of LiFeBO_3 material. Various amount of fluorine are given during preparation to reach optimum electrochemical performance. The structure of anion doped LiFeBO_3 are investigated by X-ray diffraction, ^7Li magic angle spinning NMR spectroscopy, and Fourier Transform Infrared spectroscopy. Also, the electrochemical test and cyclic voltammetry are performed by galvanostatic charge and discharge test. The result showed that fluorine-doped LiFeBO_3 has effectively improved electrochemical performance.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 09:56

Chair: Jongwoo Lim (Seoul National University)

Preparation of lithium iron pyrophosphate as cathode material for lithium ion battery

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Lithium-ion batteries are the most important energy storage system for wide applications in electronic portable devices and electric vehicles. Among cathode materials, the olivine structured lithium iron phosphate (LiFePO_4), has low cost, low toxicity, high thermal stability and high relatively high theoretical specific capacity. However, its poor high-rate performance of this material restricts its use in large-scale application owing to its low electronic conductivity and slow lithium-ion diffusion. As an alternative cathode material, $\text{Li}_2\text{FeP}_2\text{O}_7$ consisted by pyrophosphate (P_2O_7)⁴⁻ is driven by their thermal stability and improved safety. Pyrophosphate has a two-dimensional lithium diffusion channel and capability to extract more than one lithium ion per formula unit. Iron-based pyrophosphate has cyclic voltammetry (CV) peaks that appear $\text{Fe}^{2+}/\text{Fe}^{3+}$ redox couple at the range of 3.5 ~ 4.0V. In this study, anion doping like fluorine anion is adopted to improve the electrochemical property through the improvement of conductivity. The electrochemical properties of samples were investigated through lithium extraction/inserting processes using galvano-static charge/discharge and CV measurements to investigate for Li^+ transferring between the electrode materials. Also, solid-state ^7Li NMR have been observed to characterize the structural transformation.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:00

Chair: Jongwoo Lim (Seoul National University)

HPLC-UV Determiation of Resveratrol, Oxyresveratrol and Piceatannol from Wine

Jongsung Noh, JinSol Lee, Won Hoe Koo, 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 (DES-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, volume of acetic, anhydride, time of derivatization, type of basic solution for derivatization, and the effect of salt. Chromatographic separation with HPLC/UV-vis was performed using the Innoval ODS-2 (4.6 mm id × 150 mm length, 5 μm particle size) column and gradient elution mode using water and methanol.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:04

Chair: Jongwoo Lim (Seoul National University)

Facile method to fabricate viscoelastic nanocomposites based on supramolecular gels and boron nitride nanotubes via one-pot melt-blending

TaeHyeong Kim, Seunghyun Lee*

Department of Nanochemistry, Gachon University, Korea

We herein report a facile, cost-competitive, and scalable method for producing viscoelastic nanocomposites using supramolecular gels and boron nitride nanotubes (BNNTs) in polymer matrix. by simple mixing. Unlike carbon nanotubes (CNTs), BNNTs has been proposed as a nanocarrier and nanotransducer in the biomedical field because enhanced chemical inertia prefers biocompatibility. In addition, BNNTs demonstrates the potential for aerospace applications due to their shielding properties of strength and radiation. When mixed, a non-volatile eutectic liquid (EL) produced by brief blending of two chemical reagents with simple chemical structures. enabled not only the gelation of BNNTs (EL-BNNTs) but also the dissolution of a number of commodity polymers. To make use of these advantages, viscoelastic nanocomposites were produced via one-pot melt-blending the EL and BNNTs with polyurethane(PUR) and epoxy and their properties have been investigated

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:08

Chair: Jongwoo Lim (Seoul National University)

Metabolic profiling of plasma and urine from a randomized trial on the effects of dietary patterns.

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¹*Department of Chemistry, Sungkyunkwan University, Korea*

Habitual diet plays an important role in the metabolic profile and composition of the gut microbiota that can affect the host. To investigate the potential benefits of the Korean diet which is plant-based diet compared to western diet, we analyzed the changes of metabolites and gut microbiota after Korean diet (KD), the 2010 Dietary Guidelines for Americans (DGAD), and a typical western diet (WD). In a three-period crossover trial, 55 subjects were randomly assigned to one of six possible sequential orders for eating each diet (KD, DGAD, and WD) for 4 weeks, separated by a 2-week rest. Samples were collected before and end of each diet period. Using ¹H NMR and 16S rRNA-targeted sequencing, metabolites and gut microbiota were profiled. Multivariate analysis showed discriminated metabolic pattern between before and after samples in every diet. Pathway analyses revealed that the most enriched metabolic pathway was valine, leucine and isoleucine biosynthesis in KD; synthesis and degradation of ketone bodies in DGAD and WD. Particularly, KD decreased plasma branched-chain amino acids (BCAA), such as leucine, isoleucine, and valine, which is related to obesity metabolism. Whereas DGAD and WD increased plasma ketone bodies, such as acetate, 3-hydroxybutyrate, 2-aminobutyrate, and acetone related to lipid metabolism. Also, in correlation analysis of metabolome and gut microbiota, plasma BCAAs were negatively correlated with Bifidobacterium only after KD intervention. Trimethylamine N-oxide, betaine, and choline were positively correlated with gut microbial lipid metabolism only after WD intervention. This study demonstrates that the analysis of the host metabolism and gut microbiota provide insight into the relationship between dietary patterns and risk of metabolic disease.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:12

Chair: Jongwoo Lim (Seoul National University)

Metabolomic analysis of human blood associated with ambient particulate matter in air pollution

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Ambient particulate matter (PM) has become the major environmental risk factors in Korea, and exposure to PM is associated with adverse health effects on human. The objective of this study was to assess the alteration in response to environmental exposure and to investigate the association between levels of metabolite identified in human whole blood samples and PM with a diameter 2.5-10 μm (PM10).

In this study, we analyzed human whole blood from 457 Koreans using ^1H -NMR spectroscopy. The concentration of PM10 was used in multivariate linear regression model adjusted for age, sex, BMI, and smoking status. We found that PM10 was significantly related to energy metabolism such as lactate, pyruvate, glucose, and fumarate.

This approach can be a novel tool to identify potential biomarkers for predicting exposure of pollutants like PM10 and to assess the impacts of environmental pollution on human metabolism.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:16

Chair: Jongwoo Lim (Seoul National University)

Highly sensitive molecular diagnostics using SERS-PCR for Bacillus anthracis detection

Yixuan Wu, Younju Joung, Sohyun Park, Jaebum Choo*

Department of Chemistry, Chung-Ang University, China

The real-time polymerase chain reaction (QPCR) technique has been extensively used for the diagnosis of a wide range of infectious diseases. This technique found valuable clinical applications in the diagnosis of viral diseases but it suffers from several problems including time-consuming process and high fluorescent background noise. To resolve these problems, we developed a conceptually new surface-enhanced Raman scattering (SERS)-based PCR technique for its clinical applications. Due to its highly sensitive detection capability, it was possible to determine the concentration of target DNA in a short time by decreasing the number of PCR cycles. Consequently, SERS-PCR provides a high sensitivity and a short detection time over the conventional fluorescence-based QPCR. In the present study, we employed TaqMan-PCR to amplify a target gene, and then used the SERS detection technique for its highly sensitive detection. The combination of PCR with SERS proves to be effective for the rapid and sensitive detection of a low concentration of a target gene in a short time.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:20

Chair: Jongwoo Lim (Seoul National University)

Fabrication of PEGylated Au@Ag core-shell nanoparticles for SERS imaging of multiple biomarkers expressed on cancer cells

Namhyun Choi, Jaejeung Dang¹, Jaebum Choo^{1,*}

Department of Bionano Technology, Hanyang University, Korea

¹*Department of Chemistry, Chung-Ang University, Korea*

Implementation of the use of metal nanoparticles in cellular imaging has been recently garnered much attention. We recently developed a surface-enhanced Raman scattering (SERS)-based cellular imaging technique to detect cancer phenotype markers expressed on cell surfaces. Therein, hollow gold nanospheres (HGNs) have been used as SERS nano tags since HGNs strongly enhance the Raman signal intensity of individual nanoparticles by localized surface plasmon effects through the pin holes in the particle structures. However, this technique has some limitations including desorption of Raman reporter molecules and aggregation of HGNs in aqueous condition. To resolve these problems, polyethylene glycol (PEG)-ylated silver shell-gold hollow core nanoparticles (AgHGNs) have been fabricated and used as SERS nanotags in this work. By the silver shell encapsulation, the desorption problem of Raman reporter molecules could be solved. In addition, the SERS intensity of AgHGNs was greatly enhanced over HGNs. Then these particles were encapsulated with PEGs to make them stable in different pH, temperature and salt conditions. Finally, these PEGylated AgHGNs were used for the SERS imaging of three different tumor-associated biomarkers (CD44, EpCAM and ErbB2) expressed on breast cancer cells to confirm their multiple marker detection capability.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:24

Chair: Jongwoo Lim (Seoul National University)

SERS-based microdroplet system for high-throughput gradient analysis

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¹*Departoemt of Chemistry, Chung-Ang University, Korea*

Microfluidic technology has emerged as a highly efficient tool for the study of various chemical and biological reactions in last two decades. Recently, we reported that high-throughput biomarker detections can be achieved using a single phase gradient microfluidic channels together with surface-enhanced Raman scattering (SERS) detection. However, the deposition of nanoparticle aggregates on channel surfaces induces the “memory effect” in the continuous flow regime, thus affecting both sensitivity and reproducibility. To resolve this problem, a SERS-based gradient microdroplet system has been developed in this work. Herein, the sample stacking problem could be solved since two-phase liquid/liquid segmented flow reduces the memory effect. A serial dilution of a reagent could be also achieved in a stepwise manner using microfluidic concentration gradient generators. Therefore, desired concentrations of a reagent could be sequentially trapped by a small volume of droplets to prevent the sample stacking. We believe that this microdroplet system will be of significant utility in monitoring chemical and biological reactions for various concentrations of a reagent.

Oral Presentation : **ANAL2.O-23**

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:28

Chair: Jongwoo Lim (Seoul National University)

NMR structural studies of mutations in transmembrane proteins related with human diseases

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Human transmembrane proteins (hTMPs) perform essential role like gateway to permit the transport of specific substances. Additionally channel formation, cell-to-cell communication and signal transductions are also important tasks of hTMPs. The starting point for understanding and studying the specific biochemical processes of hTMPs is to determine their three-dimensional structure. The study of the structure of these membrane proteins has been extensively studied because it forms the foundation for new drugs development. The first is the transmembrane domain of amyloid precursor proteins (APP-TM) related Alzheimer's disease. What we pay attention to is the formation of amyloid channels that cause side effects such as and abnormal increase in intracellular calcium concentration. In other words, APP-TM forms a Ca²⁺ permeable ion channel in the cell membrane, destroying calcium homeostasis in normal cells, and such amyloid channels are also found in other amyloidogenic disease-related proteins such as prions and α -synuclein. The next is Syndecan-4 (Syd4), which is involved in signal transduction and cancer progression. They may affect tissue development and repair and grow factors as well as the pathogenesis of numerous diseases, especially such as cancer. The main process of action mechanism of Syd4 is the signal transmission through structural changes by ligand binding, so it is important to examine the three-dimensional structure in order to understand this process. High-purity protein samples obtained from optimized expression and purification processes have been characterized using various analytical techniques and are undergoing structural studies using solution/ solid-state NMR spectroscopy and computer modeling.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:32

Chair: Jongwoo Lim (Seoul National University)

Advanced studies of antibiotic peptides using solid-state NMR

Jinyoung Son, Yu Young Song¹, Ji-Ho Jeong¹, Yongae Kim^{1,*}

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¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

The important of adequate amounts antibiotic use can't be overestimated. Due to the abuse of classical antibiotics, antibiotic resistance has been increasing. So studies of cationic amphipathic peptides come into the spotlight as a new antibiotic. And there is still the potential for being used as candidate of good antimicrobial agent. It is also indispensable to discover new compounds to counteract the existing antibiotic resistant bacteria in the world. Lactophorin is a cationic amphipathic peptide with 23-amino acid residues derived from bovine milk. And we developed another new design to develop other novel AMPs with a more effective and less toxic antimicrobial using the sequence of the LPcin-YK3 peptide. Antimicrobial activity of designed novel AMP analogs was confirmed by bacterial killing assays and growth inhibition assays for bacteria and fungi, and the stability was confirmed by hemolysis assay and cytotoxicity assay for mouse and human eukaryotic cells. In order to understand the relationship between antibiotic function and structure of AMPs we conducted structural studies of novel AMPs using various spectroscopic methods and NMR. We successfully expressed of LPcin in E. coli and purified from the cell extract using various biophysical techniques. To confirm their 3D structures in membrane environments, we conducted solid-state NMR.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:36

Chair: Jongwoo Lim (Seoul National University)

N-Doped Carbon Dots for Dual Mode Detection with Large Dynamic Range in analysis of Ag⁺ Ion

Kim Shinik, Weekyung Kang*

Department of Chemistry, Soongsil University, Korea

Recently, carbon quantum dots have attracted attention as various advantages such as chemical inertness, lack of blinking, variable fluorescence emission, low cytotoxicity and good biocompatibility as compared with semiconductor quantum dots and organic dyes. In addition, CQD doped with heteroatoms have local surface chemical and electronic properties, thus having adjustable properties in biosensors and bioimaging. We synthesize N-doped carbon quantum dots by urea and citric acid in a single-stage microwave synthesis. The N-doped carbon quantum dots were characterized by TEM, FTIR, fluorescence spectrophotometer and uv - visible spectrophotometer. The N-CQDs exhibit fluorescence characteristics in excitation wavelength-dependent emission and strong fluorescence excitation bands are present at 360 nm and 440 nm.

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

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:40

Chair: Jongwoo Lim (Seoul National University)

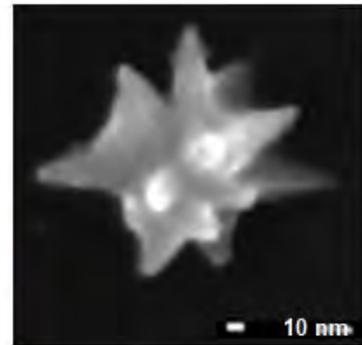
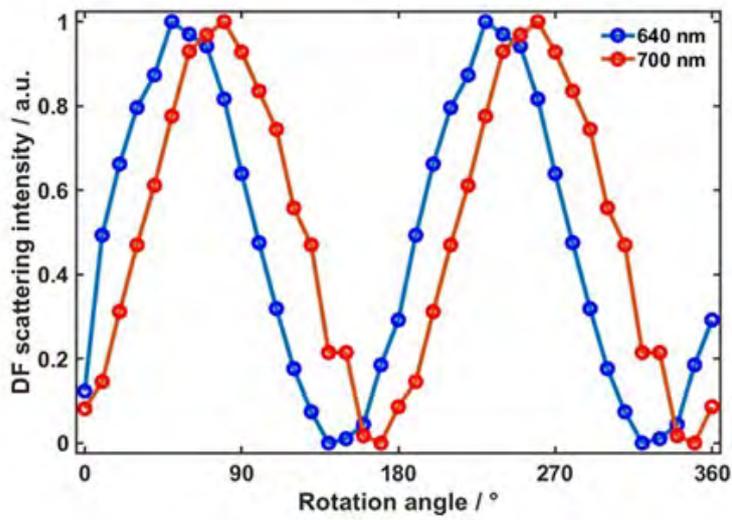
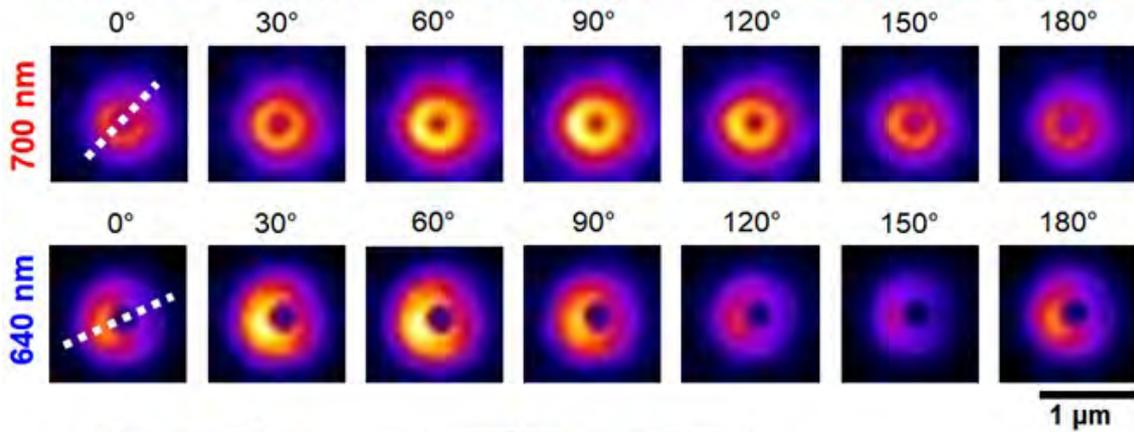
Polarization- and Wavelength-Dependent Defocused Scattering Imaging of Single Gold Nanostars with Multiple Long Branches

Geunwan Kim, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

We demonstrated the polarization- and wavelength-dependent defocused scattering properties of single gold nanostars (AuNSs) with multiple long branches on their surfaces at the localized surface plasmon resonance (LSPR) wavelengths. As a function of the rotational angle of a polarizer, the defocused DF scattering intensities of single AuNS were periodically changed without changing in the doughnut-shaped scattering patterns at two LSPR excitation wavelengths. Furthermore, the characteristic doughnut-shaped defocused scattering pattern enabled to resolve the spatial field distributions of single dipoles on the same AuNS surface at two LSPR wavelengths. Finally, we could track real-time rotational dynamics of a AuNS rotating on a glass slide under defocused microscopy. Therefore, we provided a deeper understanding of the defocused scattering properties of single AuNSs with multiple long branches randomly extended on the surface.

Polarization-dependent Defocused Images of Gold Nanostar



Oral Presentation : **ANAL2.O-27**

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:44

Chair: Jongwoo Lim (Seoul National University)

Accurate measurement of total arsenic by considering arsenic species

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

Department of Chemistry, Mokpo National University, Korea

Accurate measurement of total arsenic in a sample has been important as the toxicity related to the arsenic element has been widely known. Total amount of arsenic in a sample has been critical, but the chemical species of arsenic has also been very critical because their toxicity depend on the chemical forms. However, 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. For the quantitation of total arsenic in a sample, arsenic species in a sample have been not considered as far as we know. In general, the standard solution of arsenic has been made by As(V) standard. It might be good for the sample which its major species are As(V). But, if the major species of arsenic in a sample are different from As(V), the arsenic species of the standard solution 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 different arsenic species used in this study were As(V), As(III), MMA, DMA and AsB. The internal standards for the determination of total arsenic in rice and oyster were also investigated in this study. The best internal standard was Tellurium.

Oral Presentation : **ANAL2.O-28**

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:48

Chair: Jongwoo Lim (Seoul National University)

Influence of the Capping Material on Chemical Interface Damping Induced by Pyridine with Nitrogen in Single Gold Nanorods

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The chemical interface damping (CID) is one of the plasmon decay processes in gold nanoparticles. Herein, to find new functional groups that can induce CID as an alternative to thiol groups, we performed dark-field (DF) scattering studies of gold nanorods (AuNRs) with pyridine as adsorbate. We found that the adsorption of pyridine molecules on single AuNRs through a Nitrogen-Au interaction leads to the increased localized surface plasmon resonance (LSPR) linewidth. However, pyridine molecules were not adsorbed effectively on the AuNR surfaces with the capping reagent on the particle surfaces. Therefore, this study allows us to gain new understanding of the effect and role of the capping reagent in CID induced by pyridine. Furthermore, pyridine with nitrogen, an alternative to thiol groups, was revealed to induce a strong CID in AuNRs through the interaction of nitrogen with the Au surfaces where the capping material was removed by the oxygen plasma treatment.

Oral Presentation : **ANAL2.O-29**

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:52

Chair: Jongwoo Lim (Seoul National University)

Shape Effect on the Refractive Index Sensitivity of Localized Surface Plasmon Resonance Inflection Points in Single Gold Nanocubes with Vertices

Ji Won Ha*, **Hui Bin Jeon**

Department of Chemistry, University of Ulsan, Korea

Plasmonic gold nanoparticles with sharp tips and vertices, such as gold bipyramids (AuBPs) and gold nanocubes (AuNCs), have been widely used for high-sensitivity localized surface plasmon resonance (LSPR) sensing. However, conventional LSPR sensors based on frequency shifts have a major disadvantage: the asymmetry and broadening of LSPR peaks because of instrumental, environmental, and chemical noises that limit the precise determination of shift positions. Herein, we demonstrated an alternative method to improve the efficiency of the sensors by focusing on homogeneous LSPR scattering inflection points (IFs) of single gold nanoparticles with a single resonant mode. In addition, we investigated the effect of the shape and vertices of AuNCs on the refractive index (RI) sensitivity of homogeneous LSPR IFs by comparing with gold nanospheres (AuNSs) of similar size. The results show that for both AuNCs and AuNSs, tracking homogeneous LSPR IFs allows for higher RI sensitivity than tracking the frequency shifts of the LSPR peaks. Furthermore, single AuNCs with vertices exhibited higher RI sensitivity than single AuNSs of similar size in the homogeneous LSPR IFs. Therefore, we provided a deeper insight into the RI sensitivity of homogeneous LSPR IFs of AuNCs with vertices for their use in LSPR-based biosensors.

Oral Presentation : **ANAL2.O-30**

Oral Presentation of Young Analytical Chemists II

Room 202, FRI 10:56

Chair: Jongwoo Lim (Seoul National University)

Metal Dopants Effect on the electronic structures of $M_2Au_{36}(SR)_{24}(M=Pt, Pd)$

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 : **LIFE.O-1**

Oral Presentation of Young Life Chemist

Room 303, THU 09:00

Chair: Hyun Soo Lee (Sogang University)

Nitric Oxide-Scavenging Nanogel for Treating Rheumatoid Arthritis

Jiwon Yeo, Junseok Lee¹, Won jong Kim^{2,*}

Chemistry, Pohang University of Science and Technology, Korea

¹*Pohang University of Science and Technology, Korea*

²*Department of Chemistry, Pohang University of Science and Technology, Korea*

Nitric oxide (NO), a radical gas molecule produced by nitric oxide synthase (NOS), plays a key role in the human body. However, when endogenous NO is overproduced by physiological disorders, severe inflammatory diseases such as rheumatoid arthritis (RA) can occur. Therefore, scavenging NO may be an alternative strategy for treating inflammatory disorders. In our previous study, we developed a NO-responsive macro-sized hydrogel by incorporating an NO-cleavable crosslinker (NOCCL); here, we further evaluated the effectiveness of the NO-scavenging nano-sized hydrogel (NO-Scv gel) for treating RA. NO-Scv gel was simply prepared by solution polymerization between acrylamide (Am) and NOCCL. When the NO-Scv gel was exposed to NO, NOCCL was readily cleaved by consuming the NO molecule, as demonstrated in a Griess assay. As expected, the NO-Scv gel reduced inflammation levels by scavenging NO in vitro and showed excellent biocompatibility. Furthermore, the more promising therapeutic effect of the NO-Scv gel in suppressing the onset of RA was observed in vivo in a mouse RA model and compared to the effects of dexamethasone, a commercial drug. Therefore, our findings suggest the potential of the NO-Scv gel for biomedical applications and further clinical translation.

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

Oral Presentation of Young Life Chemist

Room 303, THU 09:15

Chair: Hyun Soo Lee (Sogang University)

Development and Application of Fluorescent Nucleoside Analogues

Shingo Hirashima, Ji Hoon Han, Soyoung Park*, Hiroshi Sugiyama*

Chemistry, Kyoto University, Japan

Fluorescent nucleoside analogues have received much attention as powerful tools for chemical biology. Their applications have expanded our understanding of biological phenomena by visualizing DNA. Previously, we have developed fluorescent guanosine analogue, thG. It can be readily applied in solid-phase synthesis; moreover, its triphosphate was enzymatically incorporated into DNA through PCR amplification. We visualized structural change of DNA from right-handed B-form to left-handed Z-form using its highly emissive property.^{1,2} Furthermore, we developed new FRET system using thG as a donor and tC as an acceptor. In this system, FRET efficiency depends on both distance and orientation factor because the fluorophores are strictly fixed in double helix structure. We introduced this system into nucleosomal DNA and demonstrated that isomorphic nucleobase FRET system could be useful for studying nucleosome structure and its dynamics.^{3,4} Very recently, we have synthesized a new fluorescent thymidine analogue, ^{diox}T. It exhibits high affinity with adenine as thymine surrogate and relatively high quantum yield in DNA duplex. Now, we are studying the construction of FRET system which consists of ^{diox}T and tC. In this presentation, I introduce our research on fluorescent nucleosides.

- 1) Park, S. et al. *Chem. Commun.* **2014**, 50, 1573.
- 2) Otomo, H. et al. *RSC Adv.* **2014**, 4, 31341.
- 3) Han, J. H. et al. *Chem. Eur. J.* **2017**, 23, 7607.
- 4) Han, J. H. et al. *Chem. Eur. J.* **2018**, 27, 17091.
- 5) Wilhelmsson, L. M. et al. *J. Phys. Chem. B.* **2003**, 107, 9094.

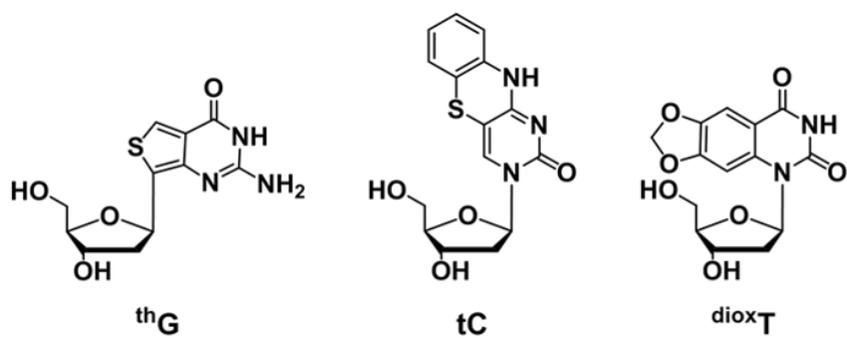


Figure 1. Chemical structure of thG, tC,⁵ and ^{diox}T.

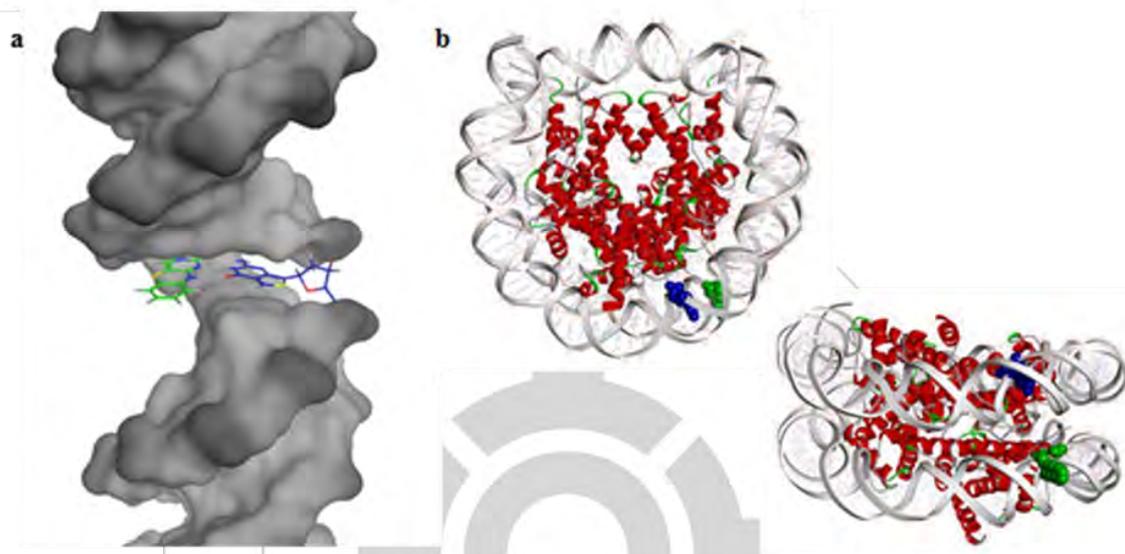


Figure 2. Schematic illustration of thG-tC FRET pair in (a) double-stranded DNA and (b) nucleosome (top view and side view)



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

Oral Presentation of Young Life Chemist

Room 303, THU 09:30

Chair: Hyun Soo Lee (Sogang University)

Structural basis for low catalytic activities in the two minor β -carbonic anhydrases from the filamentous fungi *Aspergillus fumigatus*

Songwon Kim, Mi Sun Jin^{1,*}

School of Life Sciences, Gwangju Institute of Science and Technology, Korea

¹*Division of Life Science, Gwangju Institute of Science and Technology, Korea*

In the fungal kingdom, the β -carbonic anhydrases (β -CAs) are widely distributed zinc-metalloenzymes that play essential roles in growth, survival, development and virulence. In particular, the majority of filamentous ascomycetes possess multiple β -CA isoforms in which the majors and minors have been characterized. Herein, we tested for in vitro catalytic behaviors of the two minor β -CAs, CafC and CafD, from *Aspergillus fumigatus*, and confirmed that both enzymes exhibit low CO₂ hydration activities. To understand the structural basis of their low activities, we further performed X-ray crystallographic and site-directed mutagenesis studies. Both enzymes exist as homodimer. Similar to other Type-I β -CAs, CafC active site reveals the “open” conformation in which the zinc ion is tetrahedrally coordinated by three residues (C36, H88 and C91) and a water molecule. However, L25 and L78 on the rim of the catalytic entry site protrude into the active site cleft, partially occluding access to it. Consistent with our structural analysis, single (L25G or L78G) and double mutants provide functional evidences that widening the entrance to the active site greatly accelerates the catalytic reaction. By contrast, CafD shows a typical Type-II “closed” conformation in which a zinc-bound water is replaced by aspartic acid (D36). The most likely explanation of this result is that a completely conserved arginine within the β -CA family is substituted to glycine (G38), therefore, D36 is not allowed to undergo a conformational change by forming a D-R pair that can leave a space for a zinc-bound water and switch the enzyme to be active. Furthermore, CafD structure reveals the presence of a copper ion in the interface, which may contribute to stabilize the dimeric assembly.

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

Oral Presentation of Young Life Chemist

Room 303, THU 09:45

Chair: Hyun Soo Lee (Sogang University)

Activity of glycoengineered β -N-Acetylhexosaminidases with multiple mannose-6-phosphates in lysosomes

Hyun Jiyoung, Injae Shin*

Department of Chemistry, Yonsei University, Korea

The genetic deficiency of lysosomal β -N-acetylhexosaminidases leads to incomplete digestion of GM2-ganglioside and thus causes its progressive accumulation in lysosomes. This defect causes the onset of Tay-Sachs and Sandhoff diseases, a class of lysosomal storage disorders (LSDs). To remove GM2-ganglioside accumulated in Tay-Sachs and Sandhoff diseased cells, multiple mannose-6-phosphate (M6P)-appended β -N-acetylhexosaminidases were prepared by click chemistry between multiple M6P-containing N3-peptides and alkynylated enzymes obtained by genetic code expansion. In addition, lysosome-targeting, near-infrared (NIR)-based fluorogenic probes were synthesized and applied for (real-time) monitoring of lysosomal β -N-acetylhexosaminidase activity in cells. It was found that the multiple M6P-appended β -N-acetylhexosaminidase efficiently internalizes cells via M6P receptor-mediated endocytosis and then reaches the lysosome to regain its enzyme activity. Furthermore, the glycoengineered enzyme was able to efficiently cleave GM2-ganglioside in primary diseased cells, indicating the restoration of its activity in cells. The present strategy using the coupled genetic code expansion and biorthogonal ligation techniques is highly attractive to construct multiple M6P-containing enzymes which can be used to study LSDs.

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

Oral Presentation of Young Life Chemist

Room 303, THU 10:00

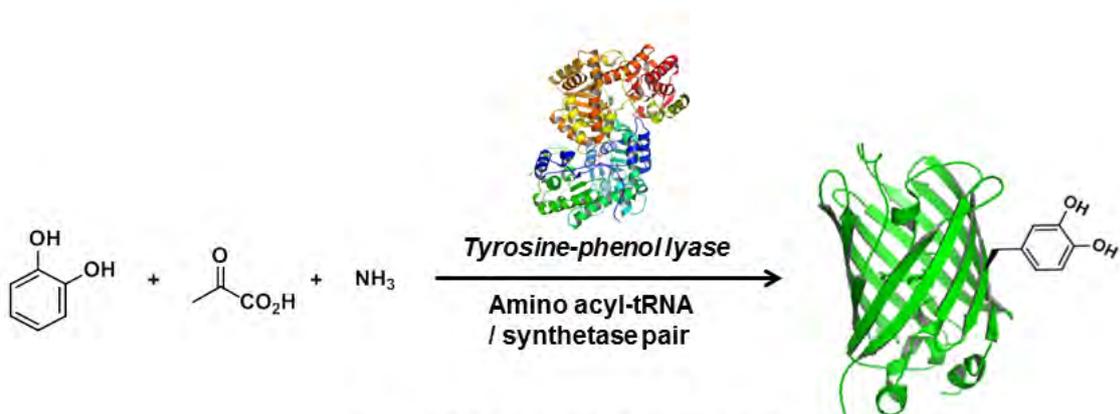
Chair: Hyun Soo Lee (Sogang University)

Genetic incorporation of L-DOPA biosynthesized by a tyrosine phenol-lyase

Sang kil Kim, Hyunsoo Lee*

Department of Chemistry, Sogang University, Korea

L-Dihydroxyphenylalanine (L-DOPA) is a naturally occurring amino acid with interesting biochemical properties. The amino acid has been used for the treatment of Parkinson's disease and various biochemical applications. In this report, L-DOPA was biosynthesized from a tyrosine phenol-lyase (TPL) by using catechol, pyruvate, and ammonia, as starting materials, and the biosynthesized amino acid directly incorporated into proteins by an evolved aminoacyl-tRNA and aminoacyl-tRNA synthetase (aaRS) pair. The aaRS used for the L-DOPA incorporation was selected from an aaRS library, and showed better efficiency than the previously reported aaRS. This direct incorporation system showed efficient L-DOPA incorporation with no incorporation of Tyr, and better protein yield than the conventional incorporation system using L-DOPA. Therefore, by using the biosynthetic system, mutant proteins containing L-DOPA could be produced with less expense and better yield. This approach could be useful for a large scale protein production for pharmaceutical and industrial application, and provide an impetus for expansion of biosynthesis of unnatural amino acids to more challenging and interesting amino acids.



Enzymatic reaction and genetic incorporation



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

Oral Presentation of Young Life Chemist

Room 303, THU 10:15

Chair: Hyun Soo Lee (Sogang University)

Forward Chemical Genetics Identified A Small-Molecule That Selectively Kill Leukemia Cells

Soobin Lee, Hyun-Suk Lim*

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

Forward chemical genetics is a highly useful strategy to explore the biological systems for chemists. In this strategy, compounds that induce a desired phenotypic change can be identified from screening a chemical library. Since it requires no hypotheses regarding the molecular basis of the phenotype in question, any genes or proteins that support this phenomenon are analyzed afterwards. The unbiased nature of the inquiry can lead to novel target proteins that could serve as novel drug targets or biomarkers, while discovering compounds that modulate those target proteins. Here, I will discuss (1) discovery of a small-molecule p27 activator that selectively kill leukemia cells, (2) identification of the target associated with the compound which may lead to the malignant behaviour of leukemia, and (3) subsequent biological studies, through forward chemical genetics. This molecule could be developed as a novel class of anti-leukemia agent, as well as a molecular tool that can provide valuable information about the role of the target in leukemia.

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

Oral Presentation of Young Life Chemist

Room 303, THU 10:30

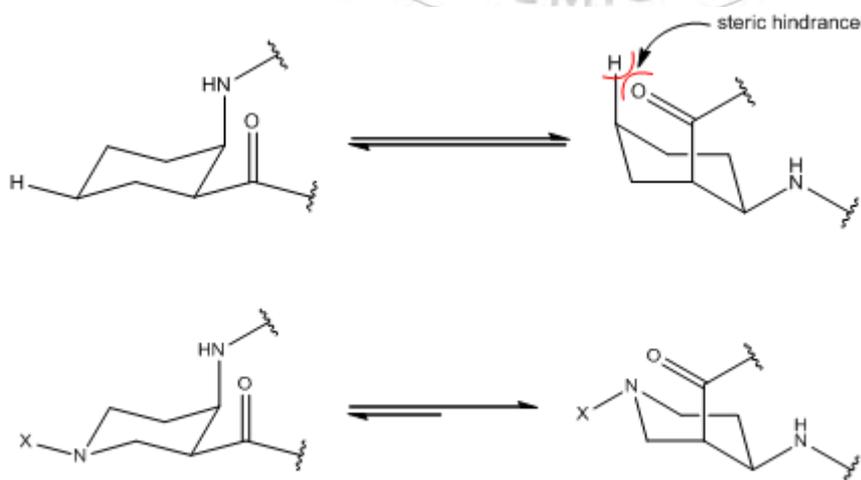
Chair: Hyun Soo Lee (Sogang University)

Research for structural characteristic change of α/β peptide oligomers containing cis-APiC

Sunglim Choi, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

Generally, we can study various helical secondary structures for synthesis of many peptide oligomers containing various residues. This research focus on α/β -peptides oligomers containing 6-membered ring β -residues because, from the previous study, we researched that α/β -peptides oligomers containing (1R,2S)-2-Aminocyclohexanecarboxylic Acid (cis-ACHC) and L-Ala have two intramolecular hydrogen bonds; $C=O(i) \cdots H-N(i+3)$ and $C=O(i) \cdots H-N(i-1)$. But in this molecule structure, we thought that axial carbonyl group at C4 in ACHC has steric hindrance because of the axial hydrogen at C6 in ACHC. Therefore using (3R, 4R)-4-Aminopiperidine-3-carboxylic acid(cis-APiC), we remove steric hindrance and expect that α/β -peptides oligomer's helix property is raised. For this research, we study with CD, IR, 2D NMR data and single crystal structure and compare with on α/β -peptides oligomers containing ACHC and Cis-AiPC protected Tosyl group in N6.



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

Oral Presentation of Young Life Chemist

Room 303, THU 10:45

Chair: Hyun Soo Lee (Sogang University)

Seeing DNA Sequences: Fluorescent Polypyrrole for A/T Sequence Visualization on Single DNA Molecules

Seonghyun Lee, Kyubong Jo*

Department of Chemistry, Sogang University, Korea

Fluorophore-linked, sequence-specific DNA binding reagents can visualize sequence information on a large DNA molecule. In this talk, we synthesized newly designed TAMRA-linked polypyrrole to visualize adenine and thymine base pairs. A fluorescent image of the stained DNA molecule generates an intensity profile based on A/T frequency, revealing a characteristic sequence composition pattern. Computer-aided comparison of this intensity pattern with the genome sequence allowed us to determine the DNA sequence on a visualized DNA molecule from possible intensity profile pattern candidates for a given genome. Moreover, TAMRA-polypyrrole offers robust advantages for single DNA molecule detection: no fluorophore-mediated photocleavage and no structural deformation, since it exhibits a sequence-specific pattern alone without the use of intercalating dyes such as YOYO-1. Accordingly, we were able to identify genomic DNA fragments from *E. coli* cells by aligning them to the genomic A/T frequency map based on TAMRA-polypyrrole-generated intensity profiles.

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 09:00

Chair: Jun Hee Lee (Dongguk University)

Visible Light-induced Photoredox-catalyzed Regioselective allylation of Activated Alkenes

Arjun Gontala^{*}, Sang Kook Woo^{1,*}

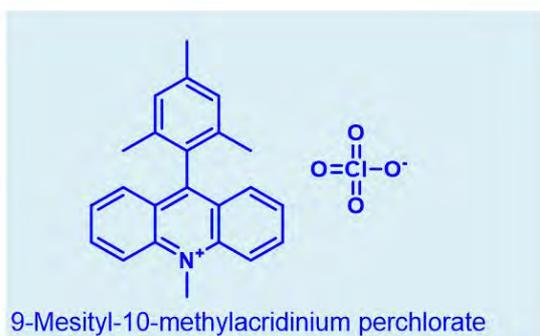
Department Of Chemistry, University Of Ulsan, Korea

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

Highly regioselective allylation of activated alkenes achieved via visible-light mediated metal-free photoredox-catalysis. The reaction involves in situ generated allylic radicals from allylsilanes via photoinduced single electron transfer (SET) mechanism, which subsequently adds regioselectively to the activated alkenes. The reaction works at ambient temperature in metal-free condition, with no extra additives, tolerates various functional groups and present wider substrate scope. The reaction is also feasible on a gram scale. Allylated products serve as a useful reactive set that can undergo a various synthetic transformation.



24 substrates,
55-87 % yield



- Metal free
- No external additives
- Redox Economical
- Ambient Condition

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 09:15

Chair: Jun Hee Lee (Dongguk University)

Total Syntheses of (+)-Uleine and (-)-Tubifolidine via Kinetically Controlled Fischer Indole Synthesis

Dong-Hyun Kim, Cheon-Gyu Cho*

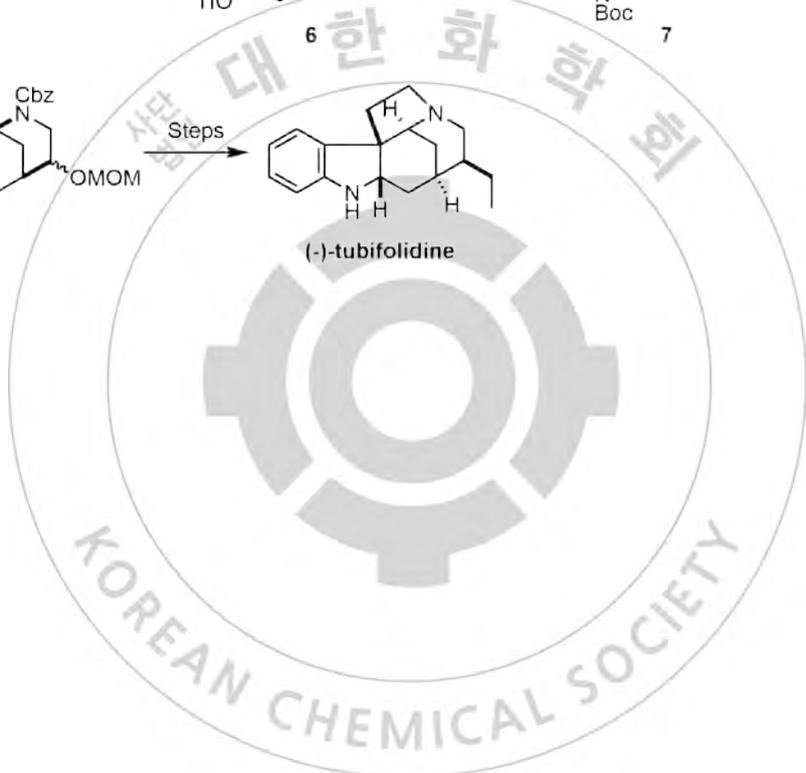
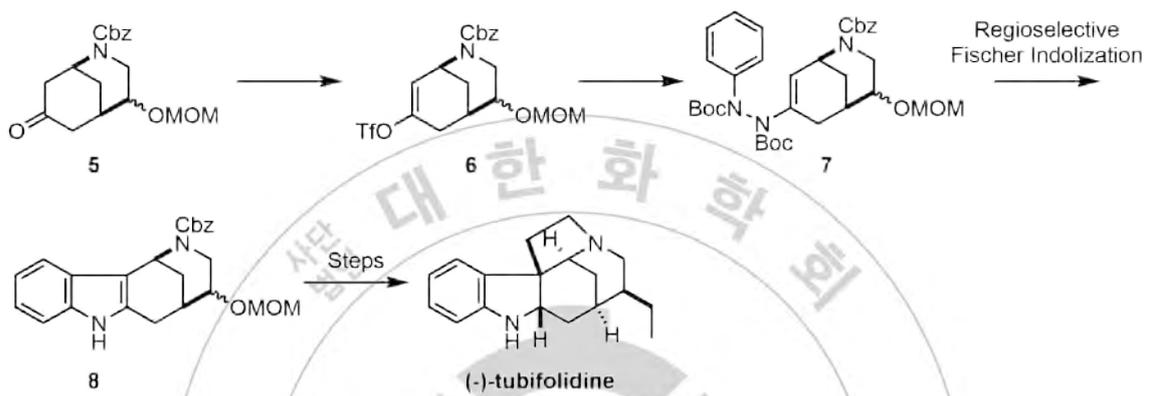
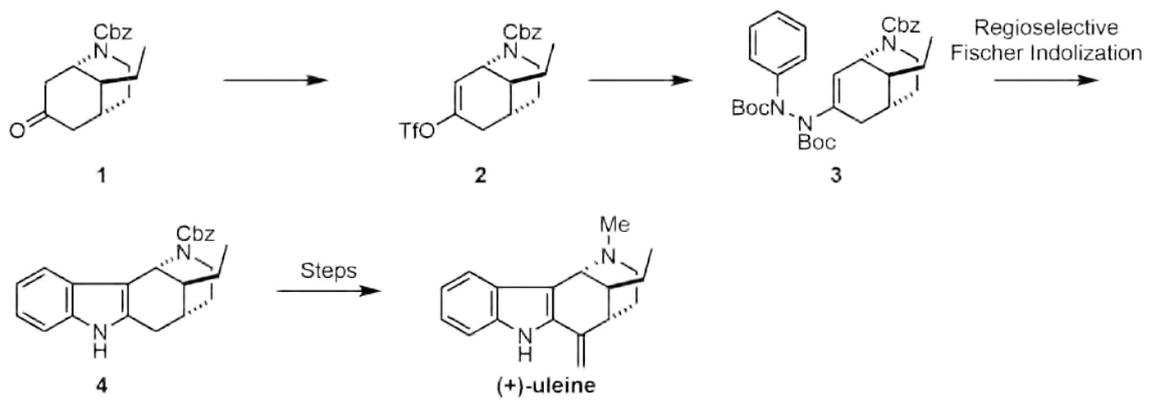
Department of Chemistry, Hanyang University, Korea

We have previously reported the synthesis of ene-hydrazone from enol triflate and subsequent indolization reaction as a new entry to a 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-hydrazone. 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 (+)-uleine and (-)-tubifolidine by ways of bicyclic carbamates **1** and **5**. Formation of enol triflates **2** and **6** followed by C-N coupling reactions with phenyl hydrazide and regioselective Fischer indolization under Lewis acidic conditions would selectively give desired indole **4** and **8**, respectively. Our recent progress on the total syntheses of (+)-uleine and (-)-tubifolidine will be presented.

References

1. Lim, B.-Y.; Jung, B.-E.; Cho, C.-G. *Org. Lett.* **2014**, *16*, 4492-4495.
2. Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.* **2017**, *19*, 6168-6171.



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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 09:30

Chair: Jun Hee Lee (Dongguk University)

Memory of Chirality approach to the asymmetric total synthesis of Salinosporamide B

Soojun Park, Sanghee Kim^{1,*}

College of Pharmacy, Seoul National University, Korea

¹*College of Pharmacy / Department of Pharmacy, Seoul National University, Korea*

The term, “Memory of Chirality (MOC)”, describes a phenomenon in which the chirality of the starting material is preserved in a reactive intermediate for a limited time. Although MOC is an attractive strategy for asymmetric synthesis, only a few applications of MOC to total synthesis have been reported. Using the principles of MOC, we performed a concise asymmetric total synthesis of Salinosporamide B. Our key step, one-pot intramolecular Aldol reaction and hydrolysis, proceeded with a high level of chirality preservation and complete diastereoselectivity without the aid of external chiral sources. To finalize the total synthesis, we also focused on one-pot oxidation and Barbier type addition after lactam ring formation step. This study represents a significant advance in the synthetic utility of MOC.

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 09:45

Chair: Jun Hee Lee (Dongguk University)

Development of novel carbapenem-based fluorogenic probe for specific detection of carbapenemase-expressing bacteria

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*

Carbapenem, one of the important clinically available antibiotics, is effective in treating infection of gram-negative bacteria due to its broad activity against bacterial pathogens and excellent stability against most β -lactamases. However, carbapenem-resistance enterobacteriaceae (CREs) have been frequently observed in these days. Therefore, the burden of carbapenem resistance is increasing and becoming a major public health crisis worldwide. A primary mechanism of carbapenem resistant among the carbapenemase-producing organisms (CPOs) is including acquisition/expression of carbapenemase, which hydrolyzes the amide bond of the β -lactam ring specifically. Several cases of CREs therapeutic failure have been reported due to the poor susceptibility of carbapenemase inhibitors and rapid transmission of carbapenemase by plasmid in CREs. Accordingly, development of efficient and accurate detection method of CREs is required for infection control and guidance. Current methods for the detection of CREs can be categorized into phenotypic and genotypic methods. Although many studies have been reported on phenotypic methods that are more widely used than expensive genotypic methods, they are still time-consuming and lack sensitivity and specificity. Very recently, activity-based detection methods have been developed to overcome these disadvantages. In particular, fluorescence-based assays have attracted attention owing to relatively low cost, high sensitivity and operational simplicity. In this study, we report synthesis and evaluation of novel fluorogenic carbapenemase substrates for the specific detection of the CPOs. These probes consist of carbapenem core structure, cleavable linkers and fluorescence dyes, which can turn on fluorescence upon hydrolysis by carbapenemase. The result from clinical assessment of our new probes demonstrated that they would be applicable to practical assays to rapid and accurate detection of the CPOs for timely diagnosis and treatment of infected patients.

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 10:00

Chair: Jun Hee Lee (Dongguk University)

A New Approach to Polarity Probe for Quantitative Intracellular Imaging

Sang Jun Park, Hwan Myung Kim*

Department of Energy Systems Research, Ajou University, Korea

Cell homeostasis is maintained by various factors such as viscosity, polarity, temperature and pH which controls the transport and diffusion of substances inside and outside the cell, and interactions between substances. Among them, intracellular polarity is an important parameter that promotes various cellular processes such as differentiation, local membrane growth, activation of the immune response, directional cell migration, and vector transport of molecules across the cell layer. The pathological activity of the cell changes the cell polarity, especially abnormal polarity is directly related to cancer. Thus, detecting of the cell polarity is essential for monitoring the status of each cell. The polarity of a typical solution can be detected with a commercial polarity meter. However, the only way to detect the intracellular polarity is detection using fluorescent probes. Most reported polarity probes have a turn-on system when they are protonated at intramolecular carbonyl groups in polar environment. Another system is ICT-based probes that is changed of the fluorescence wavelength due to polarity change. These probes are located in each organelle of the cells, showing the polarity of the microenvironment. We developed a ratiometric polarity probe with an intramolecular cyclization-opening system, depending on the polarity, unlike conventional methods. This probe is located in various intracellular regions as well as specific organelles in the cell and shows the distribution of the polarity of various regions within the cell.

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 10:15

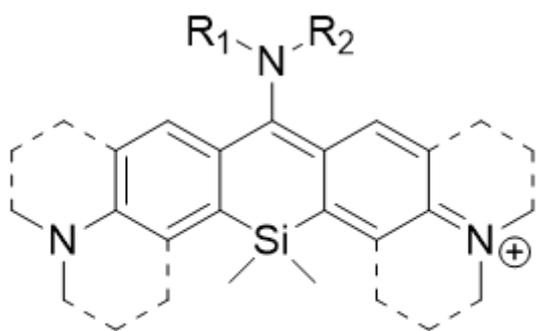
Chair: Jun Hee Lee (Dongguk University)

Development of Far-red/NIR Emitting, Two-Photon Absorbing Amino-Si-Pyronin Dyes

Kyeong Hwan Kim, Kyo Han Ahn*

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

Far-red/NIR emitting organic fluorophores are in great demand for microscopic tissue and whole-body imaging with minimal autofluorescence and reduced light scattering. Currently, only a few classes of far-red/NIR fluorophores are available. Herein, we present novel classes of far-red/NIR-emitting dyes that are photo-stable, very bright, biocompatible, and also two-photon absorbing. Introduction of an electron-withdrawing group on the C-10-amino substituent of amino-Si-pyronin dyes (aASiP) caused huge bathochromic shifts, leading to the NIR-emitting amino-Si-pyronin dyes (NIR-aASiP). However, the NIR-aASiP dyes showed very dim cellular images in the far-red/NIR wavelength region but strong emission in the shorter wavelength (yellow) region. The unexpected cellular imaging results indicated chemical instability inside cells, which is plausibly caused by nucleophilic attack of biomolecules (biothiols or amines). This biostability issue was solved by converting acyclic amine donor into julolidine-derived donor that increases the electron density at C-10 and thus protects it from nucleophilic attack by the biomolecules. The julolidine-derived NIR-emitting amino-Si-pyronin dyes (NIR-jASiP) have high cellular stability as well as two-photon absorbing property. The far-red and NIR emitting amino-Si-pyronin dyes constitute a promising fluorescence resonance-energy transfer (FRET) system and both dyes have great potential for biomedical imaging application



$R_1 = \text{alkyl}; R_2 = \text{H, COR}', \text{CO}_2\text{R}'$



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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 10:30

Chair: Jun Hee Lee (Dongguk University)

Synthesis of functional brush polymers by post-polymerization modification: transesterification approach

Lee Nam joo, Jeung Gon Kim^{1,*}

Department of chemistry, Chonbuk National University, Korea

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

Bottlebrush polymers are three dimensional soft materials of great interest. The compact and confined structures endow unique properties, which other polymers could not have. Various synthetic methods have been developed. However, the synthesis of a group of functional brush polymers with uniform structure have not been achieved. We hypothesize that post-polymerization modification method on brush polymers would upgrade the level of precision of this area. As a model, we have worked on the synthesis of acrylate macromonomers from post-modification of poly methyl acrylates. While the conventional acrylate macromonomers are not compatible with general polymer modification methods, our progress on new macromonomer design, its post polymerization modification, and brush polymerization will be shared in this presentation.

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

Oral Presentations for Young Scholars in Organic Division

Room 301+302, THU 10:45

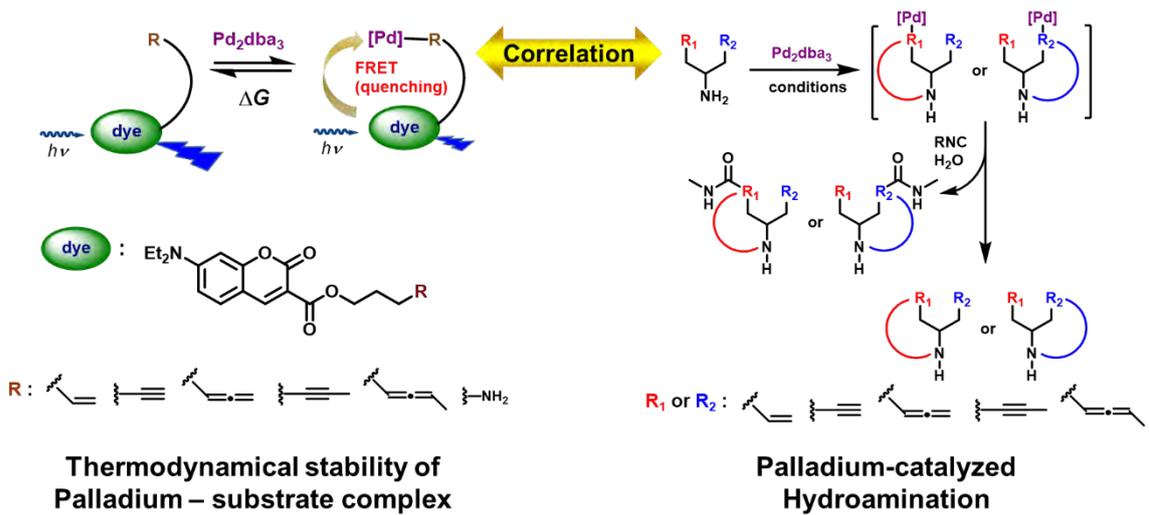
Chair: Jun Hee Lee (Dongguk University)

Selectivity among Carbon-Carbon Multiple Bonds in Palladium-Catalysed Hydroamination

Jihong Lee, Jeong-Hun Sohn*

Department of Chemistry, Chungnam National University, Korea

Carbon-carbon multiple bonds (alkenes, alkynes and allenes) are versatile functionalities for transition metal-catalysed carbon-carbon and carbon-heteroatom coupling reactions. Despite their increasing synthetic utility with recent improvements in regio- and stereoselectivity, substantial issues remain regarding selectivity among the types of C-C multiple bonds due to their relative reactivities towards a catalyst when they coexist in a reaction. Here, we present a Pd-catalysed hydroamination¹ that is highly selective for either the allene or alkyne of an aminoallenyne. We determined the relative reactivity of alkene, alkyne, allene, and amine towards the Pd catalyst using time-dependent fluorescence quenching to explain the selectivity and the reaction mechanism. Additionally, we developed a tandem reaction combining the selective hydroamination of either alkyne or allene with C-C and C-O couplings. References¹ (a) Huang, L.; Arndt, M.; Gooßen, K.; Heydt, H.; Gooßen, L. J. *Chem. Rev.* **2015**, 115, 2596-2697. (b) Muller T. E., Hultsch K. C., Yus M., Foubelo F. & Tada M. *Chem. Rev.* **108**, 3795-3892 (2008). (c) Reznichenko A. L. & Hultsch K. C. *Organic Reactions* **88**, 1-554 (2004).



Oral Presentation : **MEDIO-1**

Oral Presentation of Young Discovery Chemists

Room 304, THU 09:00

Chair: Sang Min Lim (KIST)

Discovery of Potent, Selective, and Orally Bioavailable Estrogen-Related Receptor- γ Inverse Agonists

Jina Kim, Jungwook Chin*, Sung Jin Cho*

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

ERR γ is abundantly expressed in various tissues associated with the CNS, circadian clock, and basal metabolic function; thus, it not only regulates ion homeostasis in related tissues but also controls metabolic processes such as mitochondrial biogenesis and hepatic gluconeogenesis. We synthesized potent, selective and orally bioavailable ERR γ inverse agonists and evaluated the in vitro pharmacology as well as the absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of chemical entities that not only were shown to be highly selective inverse agonists for ERR γ but also exhibited enhanced pharmacokinetic profile compared with GSK5182. We observed a significant increase of fully glycosylated NIS protein, key protein for radioiodine therapy in anaplastic thyroid cancer (ATC), in DN201000-treated CAL62 cells, which indicated that these compounds could be promising enhancers for restoring NIS protein function in ATC cells. Thus, DN201000 possess advantageous druglike properties and can be used to potentially treat various ERR γ -related disorders.

Oral Presentation : **MEDIO-2**

Oral Presentation of Young Discovery Chemists

Room 304, THU 09:15

Chair: Sang Min Lim (KIST)

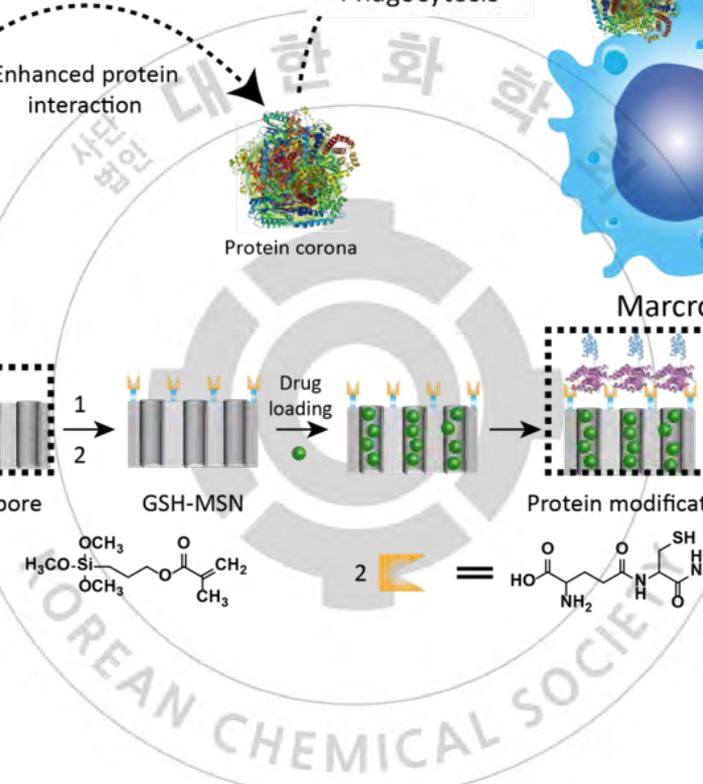
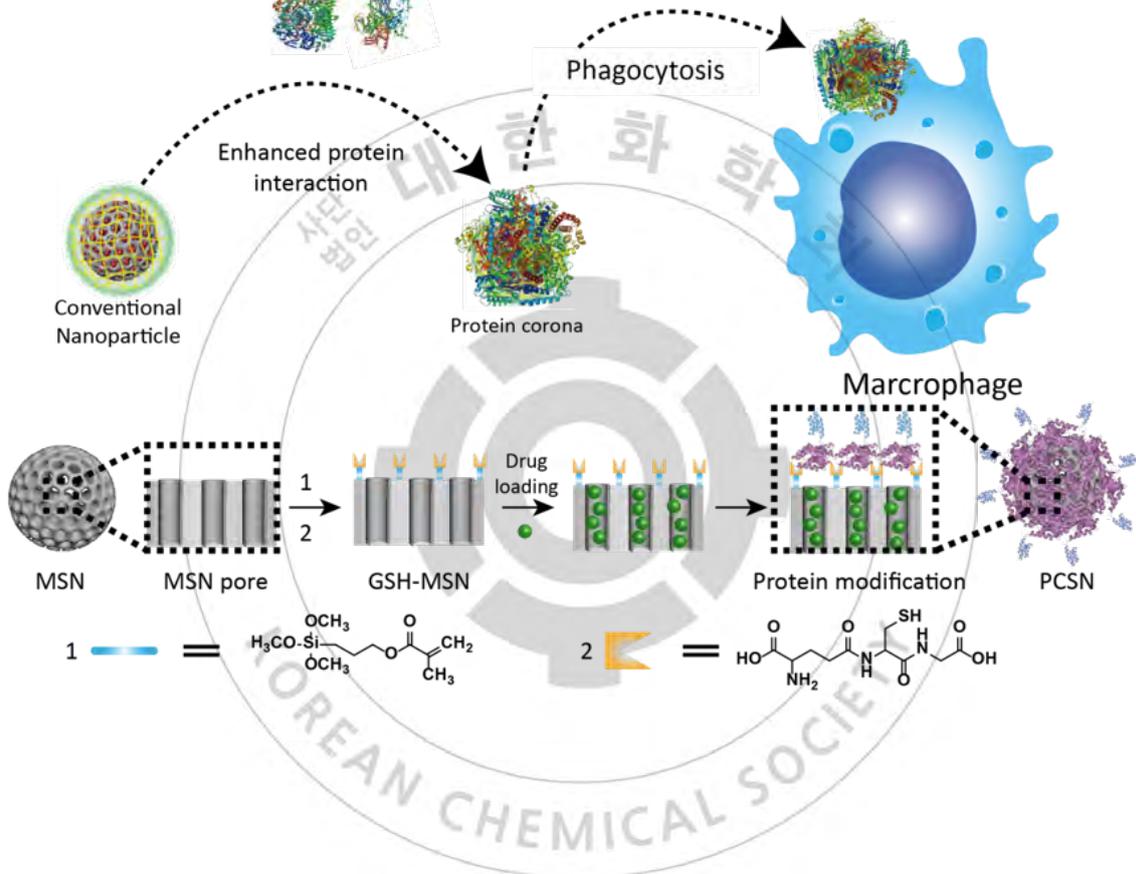
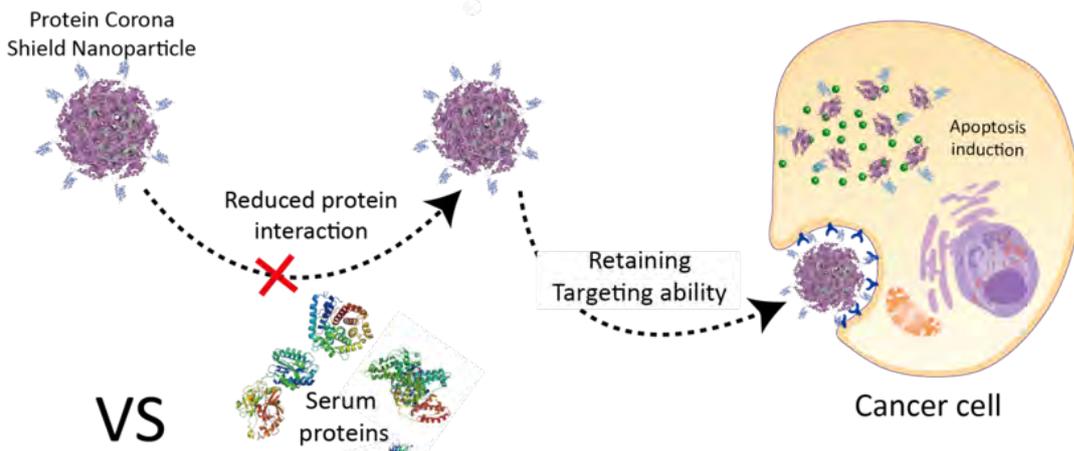
Highly efficient protein corona shield system of cloaking nanoparticles for targeted drug delivery

Jun Yong Oh, Ja-Hyoung Ryu^{1,*}

Department of Chemistry / Department of Chemical E, Ulsan National Institute of Science and Technology, Korea

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

Targeted drug delivery using nanoparticles can minimize the side effects of conventional pharmaceutical agents and enhance their efficacy. However, translating nanoparticle-based agents into clinical applications still remains a challenge due to the difficulty in regulating interactions on the interfaces between nanoparticles and biological systems. Here, we present a targeting strategy for nanoparticles incorporated with a supramolecularly pre-coated recombinant fusion protein in which HER2-binding affibody combines with glutathione-S-transferase. Once thermodynamically stabilized in preferred orientations on the nanoparticles, the adsorbed fusion proteins as a corona minimize interactions with serum proteins to prevent the clearance of nanoparticles by macrophages, while ensuring systematic targeting functions in vitro and in vivo. This study provides insight into the use of the supramolecularly built protein corona shield as a targeting agent through regulating the interfaces between nanoparticles and biological systems.



Oral Presentation : **MEDIO-3**

Oral Presentation of Young Discovery Chemists

Room 304, THU 09:30

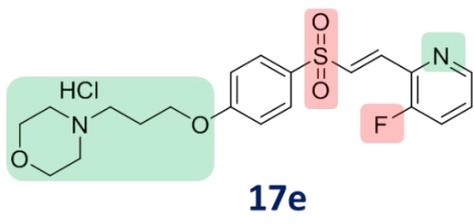
Chair: Sang Min Lim (KIST)

Design, Synthesis and Optimization of Novel Class of Nrf2 Activator as a Neuroprotective Agent for Treatment of Parkinson's disease

Ji Won Choi, Siwon Kim, Jong-Hyun Park, Hyeon Jeong Kim, Hyeon Ji Kim, Boko Jang, Sun Jun Park, Jong Seok Yoo, Areum Song, Ki Duk Park*

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

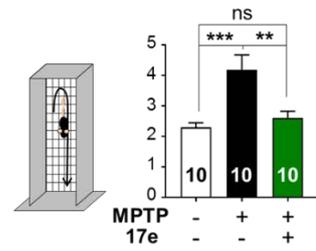
We previously developed a novel series of vinyl sulfones as nuclear factor erythroid 2-related factor 2 (Nrf2) activators with therapeutic potential for Parkinson's disease (PD). However, the previously developed lead compound (**1**) exhibited undesirable drug-like properties. Here, we optimized vinyl sulfones by introducing nitrogen heterocycles to improve drug-like properties. Among the synthesized compounds, **17e** was the most promising drug candidate with good drug-like properties. Compound **17e** showed superior effects on Nrf2 activation in cell-based assays compared to compound **1** (**17e**: EC₅₀ = 346 nM; **1**: EC₅₀ = 530 nM). Compound **17e** was further confirmed to induce expression of Nrf2-dependent antioxidant enzymes at both mRNA and protein levels. In a 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP)-induced mouse model of PD, **17e** significantly attenuated loss of tyrosine hydroxylase-immunopositive dopaminergic neurons, suppressed microglial activation, and alleviated PD-associated motor dysfunction. Thus, **17e** is a novel Nrf2 activator with excellent drug-like properties and represents a potential therapeutic candidate for PD.



Activity & Drug-Like Properties

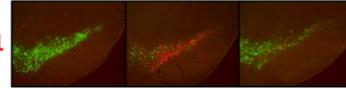
**Nrf2
Activation**

PD model



MPTP
17e

TH & Iba1



Oral Presentation : **MEDIO-4**

Oral Presentation of Young Discovery Chemists

Room 304, THU 09:45

Chair: Sang Min Lim (KIST)

Novel tau aggregation inhibitors for treatment of Alzheimer's Disease

WooSeung Son, Sang Min Lim¹, Kyu-Sung Jeong, Ae Nim Pae^{1,*}

Department of Chemistry, Yonsei University, Korea

¹Convergence Research Center For Diagnosis, Treatment and Care System of Dementia, Korea Institute of Science and Technology, Korea

Alzheimer's disease(AD) is a chronic neurodegenerative disease that is the most common form of dementia. It is still unknown what AD causes, but AD features two histopathological hallmarks : amyloid plaques(AP) made of amyloid- β and neurofibrillary tangles(NFTs) arising from the hyperphosphorylated tau aggregation in pathology. It is known AP and NFT are neurotoxic that may lead to impairment of brain. In clinical trials, diverse compounds, such as amyloid aggregation inhibitors, β -secretase inhibitors and so on, have been failed to cure AD patients. Therefore, our rationale of tau aggregation inhibitors reduce the generation of NFT that may relate to causes of AD. We identified lead compound (DTC0100) which inhibits tau aggregation by high contents screening in Tau Bi-FC cell-based assays. Then, a variety of derivatives were synthesized through a structure-activity relationship study and the optimization of novel tau aggregation inhibitors to improve potency, physicochemical properties and in vivo efficacy. Among synthesized compounds, DTC0521 showed excellent inhibitory activity of tau aggregation ($IC_{50} = 0.06 \mu M$) in Tau Bi-FC assays and was also lower tau aggregation ($IC_{50} = 0.58 \mu M$) in ThS assays. DTC0521 showed the recovery of cognitive impairments (Tau-P301L-BiFC transgenic mice) in behavior test and decreases tau aggregation as well as phosphorylated tau. It also exhibited good pharmacokinetic profile and ADME/Tox, thus, the validation of DTC0521 as preclinical candidate and further optimization are in progress.

Oral Presentation : **MEDIO-5**

Oral Presentation of Young Discovery Chemists

Room 304, THU 10:00

Chair: Sang Min Lim (KIST)

Synthesis and bioevaluation of a Novel TSPO-selective PET ligand ([18F]BS224) in Animal Models of Neuroinflammation and Stroke

Sang Hee Lee, Jungmin Kim¹, Byung Chul Lee^{2,*}

Department of Transdisciplinary Studies, Graduate School of Convergence Science and Technology, Seoul National University, Suwon / Department of Nuclear Medicine, Seoul National University College of Medicine, Seoul National University Bundang Hospital, Korea

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Abnormal translocator protein 18 kDa (TSPO) expression in brain is markedly detected in activated microglia, choroid plexus, and reactive astrocytes [1]. The selective TSPO-binding ligand can provide a powerful imaging tool to detect and monitor inflammatory brain disorders, because TSPO expression is significantly lower in the normal brains [2]. Herein, we have designed an aromatic fluorine substituted imidazo[1,2-a]pyridine analogue, [18F]BS224 and presented its radio-synthesis and bioevaluation for PET imaging of neuroinflammation. Aromatic [18F]fluorination of [18F]BS224 was conducted by two different precursors and conditions: i) diaryliodonium salts by using condition A; ii) pinacol boronate ester by using condition B [4]. Finally, aromatic [18F]fluorination of [18F]BS224 was successfully optimized by nucleophilic substitution of the pinacol boronate ester precursor using [18F]fluoride with copper catalysts. The results, together with those obtained on in vitro TSPO binding, stability, in vivo PET imaging studies with specific and selective binding for TSPO, and a clear visibility of inflammatory lesion in animal models support the conclusion that [18F]BS224 is a promising TSPO PET imaging agent for neuroinflammation. Reference : [1] B. Scatton, et al. (1987) Brain research, 421, 167-172. [2] G. Kreutzberg, et al. (1997) Journal of neurocytology, 26, 77-82. [3] K. Sang Eun, et al. (2011) Organic & biomolecular chemistry, 9, 8346-8355. [4] V. Gouverneur, et al. (2014) Angewandte chemie, 126, 7885-7889.

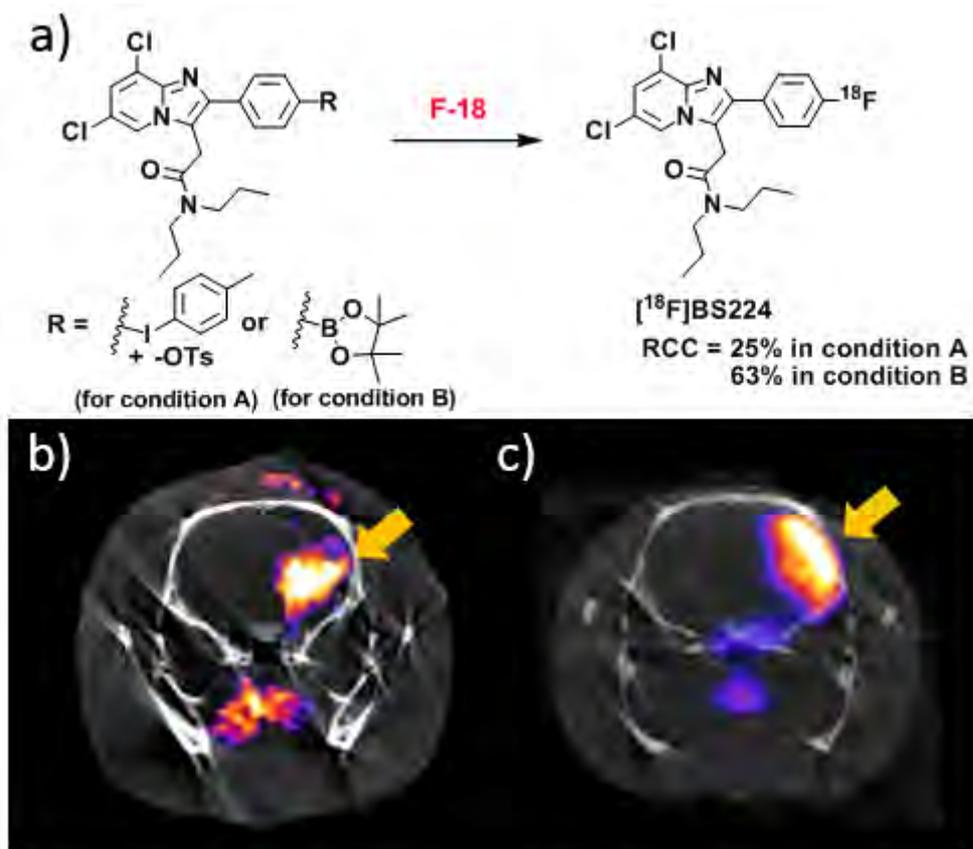


Figure. a) Radio-synthetic pathways. PET/CT axial images of $[\text{}^{18}\text{F}]\text{BS224}$ in LPS-induced b) inflammatory and c) MCAO rat models.



Oral Presentation : **MEDIO-6**

Oral Presentation of Young Discovery Chemists

Room 304, THU 10:15

Chair: Sang Min Lim (KIST)

Identification of a novel cereblon modulator and its application for PROTAC-based BET degraders

Yeong Uk Jeon, AhRa Go¹, Jae du Ha², Pilho Kim¹, Jong Yeon Hwang^{1,*}, Sung Yun Cho²

pharmacy, Sungkyunkwan University, Korea

¹*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

²*WCI, Korea Research Institute of Chemical Technology, Korea*

Immunomodulatory drugs (IMiDs) exert anti-myeloma activity by binding to the protein cereblon (CRBN) and subsequently degrading IKZF1/3. Recently, their ability to recruit E3 ubiquitin ligase has been used in the proteolysis targeting chimera (PROTAC) technology. Herein, we design and synthesize a novel IMiD analog TD-106 that induces the degradation of IKZF1/3 and inhibits the proliferation of multiple myeloma cells in vitro as well as in vivo. Moreover, we demonstrate that TD-428, which comprises TD-106 linked to a BET inhibitor, JQ1 efficiently induce BET protein degradation in the prostate cancer cell line 22Rv1. Consequently, cell proliferation is inhibited due to suppressed C-MYC transcription. These results, therefore, firmly suggest that the newly synthesized IMiD analog, TD-106, is a novel CRBN modulator that can be used for targeted protein degradation.

Oral Presentation : **MEDIO-7**

Oral Presentation of Young Discovery Chemists

Room 304, THU 10:30

Chair: Sang Min Lim (KIST)

Identification of novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

Jiwoong Lim, Ae Nim Pae^{1,*}, Sang Min Lim¹, Jae Yeol Lee², Jae Wook Lee³

Convergence Research Center for Diagnosis, Treatme, Korea Institute of Science and Technology, Korea

¹*Korea Institute of Science and Technology, Korea*

²*Department of Chemistry, Kyung Hee University, Korea*

³*Convergence Research Center for Dementia DTC, Korea Institute of Science and Technology, Korea*

SH2 domain-containing inositol 5'-phosphatase 2 (SHIP2) is a lipid phosphatase that produce phosphatidylinositol 3,4-bisphosphate (PI(3,4)P₂) from phosphatidylinositol 3,4,5-triphosphate (PI(3,4,5)P₃), and is involved in various human diseases including type 2 diabetes, cancer, and neurodegenerative diseases. A recent report demonstrated that inhibition of SHIP2 leads to functional restoration of the Akt/GSK3-dependent pathway by reducing the levels of PI(3,4)P₂. Furthermore, the fact that downregulation of the SHIP2 reduced tau hyperphosphorylation induced by amyloid β and rescued the memory impairment in a Alzheimer's disease mouse model indicates SHIP2 can be a promising therapeutic target for Alzheimer's disease. In this study, we have developed novel, potent SHIP2 inhibitors by extensive structural elaboration of hit compounds discovered from a high-throughput screening. The biological evaluation revealed that some of the synthesized compounds had good potency on SHIP2 inhibition with reasonable drug-like properties in comparison with reference compounds. Notably, one of these derivatives, compound 43, showed promising properties in an in vivo pharmacokinetic evaluation and BBB penetration study. Considering SHIP2 is one of key signal mediators for tau hyperphosphorylation, our potent SHIP2 inhibitor may function as a promising lead compound for the treatment of Alzheimer's disease.

Oral Presentation : **MEDIO-8**

Oral Presentation of Young Discovery Chemists

Room 304, THU 10:45

Chair: Sang Min Lim (KIST)

Synthesis and recent updates on thiazoline containing selective agonists of peroxisome proliferator-activated receptor δ

Tara Man Kadayat, Su-Jeong Lee, Sung Jin Cho*, Jungwook Chin*

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

Peroxisome proliferator-activated receptors (PPARs) are members of ligand-activated transcription factors of the nuclear receptor family. Based on distinct ligand specificity, physiological roles and tissue distribution, PPARs are classified into three isotypes namely PPAR α , PPAR γ , and PPAR δ . PPAR δ is considered as a promising biological target for the development of new drugs to treat metabolic syndrome including hyperlipidemia. As part of our continuous effort to develop new analogues of GW501516 (a well-known selective and potent PPAR δ agonist), we introduced a facile method for the synthesis of new thiazoline containing intermediate for the preparation of novel PPAR δ -selective agonists. The synthetic method used is short and convenient as it did not require the use of extreme conditions such as -78 °C. In this study, we developed efficient route for the synthesis of distinctive thiazoline containing compounds as selective PPAR δ agonists. These reaction conditions and unique key intermediate may be applicable for the synthesis of other related pharmaceuticals. The preliminary in vitro PPAR δ activity of synthesized compounds demonstrates this unique thiazoline core containing compounds as potential PPAR δ –selective agonist.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 09:00

Chair: Doo-Hyun Ko (Kyung Hee University)

Plasmonic nanogap engineering with DNA for biomedical application

Jeong-Wook Oh, Jwa-Min Nam^{1,*}

Department of Chemistry, Seoul National University, Korea

¹Division of Chemistry, Seoul National University, Korea

Plasmonic nanogaps can intensify electromagnetic field in their confined narrow areas, which enable to provide superior optical enhancement such as surface-enhanced Raman scattering (SERS). A narrower nanogap is more beneficial in magnifying electromagnetic field, but in fact, ~1 nm nanogap is represented as the most efficient for enhancing SERS signal due to the quantum tunneling effect. We synthesized ~1-nm plasmonic nanogap nanoparticles producing strong SERS signal. DNA-modified gold nanoparticles (AuNPs) were served as a seed, which was followed by Au growth on the seed AuNPs. ~1-nm uniform nanogap was formed with several bridges between a core AuNP and an Au shell, and we call those particles as gold-nanobridged nanogap particles (Au-NNPs). The nanogaps can be controlled by the DNA sequence and DNA grafting density. Interestingly, the exterior surface roughness of Au-NNP can induce amplification of the electromagnetic field inside the nanogap, increasing the SERS signal by ~1 order of magnitude. Due to the strong and uniform SERS effect, Au-NNPs were used as a SERS probe for biosensor and bioimaging. Herein, the synthetic mechanism and the optical properties of ultras-small nanogap inside plasmonic nanoparticles can provide valuable guidelines for developing new plasmonic nanogap structures and their biomedical applications.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 09:12

Chair: Doo-Hyun Ko (Kyung Hee University)

Iridium(III) Complexes for Deep-Red to Near-Infrared Phosphorescent Solution-Processable Organic Light-Emitting Diodes

Hae Un Kim, Seyeong Lim, Dohyun Kim, Dasol Chung, Jihyun Min, Taiho Park*

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

Research on materials and devices emitting near-infrared- (NIR-) wavelength has been driven by several application requirements. However, the development of luminophores possessing efficient, stable, low-cost NIR emission is still a challenge. Herein, in order to investigate the effects of electron-withdrawing and -donating substituents fixed on the quinoline moiety of (benzo[*b*]thiophen-2-yl)quinoline cyclometalating ligands, we developed a series of deep-red to NIR emitting iridium(III) complexes. We conducted a photophysical study at the excited-state in the solution, powder, doped polymer film and frozen matrix states to examine the effects of substitution. In doped polymer films, the $-CH_3$ substituted, unsubstituted and $-CF_3$ substituted complex were promising compounds with high phosphorescence quantum efficiency. The unoptimized device using a solution-processable method showed maximum external quantum efficiency (EQE) value of 2.11%.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 09:24

Chair: Doo-Hyun Ko (Kyung Hee University)

Novel Strategies on Preparing Ultrabright Luminescent Gold Nanoclusters via Surface Modification

Kyunglim Pyo, SangMyeong Han¹, Hongmei Xu, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

¹*department of chemistry, Yonsei University, Korea*

On account of the drastic growing interest in developing biological and optical sensing materials, preparing highly luminescent quantum-sized gold nanoclusters(AuNCs) has been one of the actively studied field for the past few decades. However, the low quantum yield(QY_{22SG18} (Au₂₂, QY~7%), via relevant surface modification. Firstly, Au₂₂ was ion-paired with bulky tetraoctylammonium(TOA) cation, which rigidified the Au(I)-thiolate shell structure by significant intermolecule interactions between the alkyl chains. This cluster was confirmed to maintain its composition, while the QY showed a mass increment of 9-fold enhanced luminescence(QY~60%). This is one of the highest QY reported yet for AuNCs. Secondly, Au₂₂ was functionalized with benzyl chloroformate and chromophores which not only rigidified the Au-thiolate shell structure by its aromatic molecules, but also induced resonance energy transfer. As a result, the luminescence increased by 8-fold compared to Au₂₂ which is similar to the TOA bound results. Moreover, this strategy remedies the drawback of the low solubility of TOA-Au in water and obtain highly luminescent water soluble AuNCs. In summary, these two approaches can be widely used to prepare various types of luminescent AuNCs tailored with functional surfaces, which will find a wide range of practical applications in biological imaging as well as luminescent displays.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 09:36

Chair: Doo-Hyun Ko (Kyung Hee University)

Microwave absorption enhancement via BaTiO₃ particles with oxygen vacancies.

Jerome Hyun*, **Baek Kyungnae¹**

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

¹*Department of Chemistry, Ewha Womans University, Korea*

Microwave absorption is important for preventing electronic malfunction in electronic devices due to electromagnetic interference. Microwave absorbing materials with high magnetic permeability or high dielectric loss are typically employed. BaTiO₃ is a ferroelectric material and can be applied as efficient microwave absorbers. The movement of the domain wall affects the dielectric properties of many ferroelectric materials in the microwave range. Microwave absorption of the ferroelectric material can be enhanced by controlling the movement of the domain wall. In this study, we used the coupling of oxygen vacancy to control the domain wall motion, thereby exploring the improvement of microwave absorption in ferroelectric BaTiO₃ particles. BaTiO_{3-x} particles were prepared by the Molten Salt Synthesis (MSS) method. Oxygen vacancies were introduced through synthesis in an oxygen deficient environment. The presence, relative concentration and predominant type of oxygen vacancies were confirmed using Raman, electron paramagnetic resonance (EPR) and Electron energy loss spectroscopy (EELS) analysis. We found that increased oxygen vacancy content by 15-folds enhanced the microwave absorption in BaTiO_{3-x} particles by 26.3dB. The calculated reflection loss value of oxygen deficient BaTiO_{3-x} particles was enhanced up to -43dB at 5GHz. From a Debye relaxation model, we attributed the increase in microwave absorption to the slowing of domain wall movement by oxygen vacancies. These results demonstrate effective control over microwave absorption using facile and cheap incorporation of oxygen vacancies in dielectric fillers.[1] K. Baek et al., "Axial oxygen-vacancy-regulated microwave absorption in micron-sized tetragonal BaTiO₃ particles" J. Mater. Chem. C, 2018, 6, 9749-9755

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 09:48

Chair: Doo-Hyun Ko (Kyung Hee University)

Direct Sensing from Self-Doped Colloidal Quantum Dots Thin-Film Transistor

Dongsun Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

Colloidal quantum dots (CQDs) have attracted much attention because of the tunability of electronic transition. Recently, the studies on the intraband transition of the CQDs, which directly uses the quantized energies in a band, are actively carried out. These studies have revealed that the intraband transition is a result of the self-doping phenomenon and are sensitive to the surface dipole change. In this presentation, I will present the self-doping properties and direct sensing mechanism of the self-doped HgSe CQD/ZnO TFT sensor. The HgSe CQDs are spin-coated over the ZnO thin-film transistor without any other receptor molecule. Surprisingly, HgSe CQD/ZnO TFT sensor had multifunctional sensitivity to the CO₂, NO, and H₂S gases, mid- IR photons, and L-cysteine molecule. To note, the CO₂ and NO gas molecules are physisorbed to the surface of HgSe CQD film and showed high reversibility in threshold voltage under a repetitive experiment. The mid-IR intraband transition of HgSe CQDs film undergoes energy transfer with the vibrational mode of gas molecules. The electronic-vibrational energy transfer (EVET) mechanism is plausible because the vibrational energy of the gas and the intraband transition have similar energy gap. On the other hand, the chemisorption result, irreversibility, is measured with H₂S gas and L-cysteine, which forms the bond between film and thiol functional group. The intraband CQDs have much potential for future sensor materials because of the easy reproductivity and low-cost fabrication process.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 10:00

Chair: Kwang Seob Jeong (Korea University)

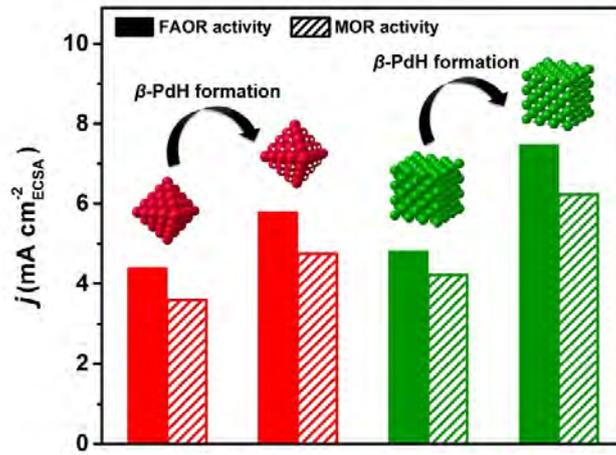
Ligand Effects of β -PdH Nanocatalysts towards the Liquid Fuel Oxidation Reaction

Jeonghyeon Kim, Sang-Il Choi^{1,*}

Kyungpook National University, Korea

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

Pd-based electrocatalysts for direct liquid fuel cells (DLFCs) have drawn significant attentions as an energy system ideal for automobile, unmanned aerial vehicles and portable electronic devices owing to their high power density. Typical strategies, including optimization of shape or facet, and composition control, have been investigated to enhance the activity and of Pd-based catalysts and study their enhanced catalysis mechanism. However, those were significant and challenging for development of advanced catalysts toward direct liquid fuel cells (DLFCs). This presentation reports the synthesis and characterization of (100)-faceted β -PdH cubes and (111)-faceted β -PdH octahedra for the first times. Those facet controlled β -PdH nanocrystals and Pd counterparts can offer an opportunity to investigate the link between the catalytic kinetics and shape/facet/composition of the catalysts. The β -PdH cubes and octahedra remarkably accelerate the catalytic activity and stability toward formic acid/methanol oxidation reaction (FAOR/MOR) due to ligand effect originated from the interstitial alloying of β -PdH. The formation and ligand effect of facet controlled β -PdH nanocrystals were confirmed by a number of techniques, including scanning transmission electron microscopy, X-ray analysis, H₂-temperature programmed reduction, and electrochemical measurements. FAOR/MOR activities of β -PdH nanocrystals and Pd counterparts are also presented.



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

Oral Presentation of Young Material Chemists

Room 405+406, THU 10:12

Chair: Kwang Seob Jeong (Korea University)

Phographene Nanosheet for High-Performance Lithium-Ion Battery Anode Applications

Siby Thomas, Sang Uck Lee^{1,*}

Department of Bio-Nano Engineering, Hanyang University, Ansan, Korea

¹*Department of Bio-Nano Engineering, Hanyang University, Korea*

The progress of eco-friendly, clean, and sustainable energy resources always demands suitable anode material for batteries with high structural stability and superior storage capacity. Herein, based on first-principles density functional theory (DFT) predictions, we systematically investigated the potential applications of α - and β phographene (PhoG) nanosheet¹ as anode material for future Lithium-ion batteries (LIBs). Our calculations show that the PhoG nanosheet possesses significant structural, electronic, and mechanical stability with high metallicity which provided enhanced conductivity for LIB application. Our results reveal that α -PhoG nanosheet show a higher theoretical specific capacity for Li atoms ($\text{Li}_{1.8}\text{C}_6$) compared to the LiC_6 of graphite and other recently reported planar carbon allotropes.²⁻⁴ We also found that both the PhoG nanosheets show fast Li mobility with a low diffusion barrier for Li atoms (< 0.30 eV) as well as low average open circuit voltage (~ 0.25 V). In view of these excellent properties, our work predicts that both the α - and β PhoG can be promising anode materials for the development of future LIBs with low-cost and high-performance. (1) Fan, X. Y.; Li, J.; Chen, G. RSC Adv 2017, 7 (28), 17417-17426. (2) Li, X. Y.; Wang, Q.; Jena, P. J Phys Chem Lett 2017, 8 (14), 3234-3241. (3) Ferguson, D.; Searles, D. J.; Hankel, M. ACS Appl Mater Inter 2017, 9 (24), 20577-20584. (4) Thomas, S.; Nam, E. B.; Lee, S. U. ACS Appl Mater Inter 2018, 10 (42), 36240-36248.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 10:24

Chair: Kwang Seob Jeong (Korea University)

Conducting Polymer Decorated Hierarchical Earth-Abundant Material as Efficient Bifunctional Electrocatalyst for Overall Water Splitting

Samiran Garain, Min Hyung Lee^{1,*}

Chemistry, Kyung Hee University, India

¹*Department of Applied Chemistry, Kyung Hee University, Korea*

Nowadays, excessive use of exhaustible fossil fuels is deemed to worsen environmental pollution and greenhouse effects. Thus, development of electrochemical hydrogen and oxygen production from water splitting is one of the most promising approaches for many modern energy storage and conversion technologies, such as fuel cells and water electrolysis, to meet the increasing global energy demands and the critical requirement of a cleaner environment. To realize the industrial applications of these energy systems, materials that drive electrocatalytic reactions with a low overpotential and a high mass activity, as well as a high durability to reduce the cost are highly desirable. In this study, the conducting polymer decorated NiCo₂S₄ as low-cost electrocatalyst shows excellent catalytic performance toward HER and OER in alkaline solution, such as super high catalytic activity, small Tafel slopes (42.2 mV dec⁻¹ for OER and 68.5 mV dec⁻¹ for HER), and superior stability, which are comparable to those of the previously reported earth-abundant material-based electrocatalysts. The catalyst exhibits very low overpotential (273 mV for OER and 77 mV for HER) to achieve a current density of 10 mA cm⁻² for HER and OER, with a promising stability over 24 hours. This work opens a new avenue for the rational design of hybrid structure catalyst towards overall water splitting for energy conversion and storage applications. This research was supported by Creative Materials Discovery Program through the National Research Foundation of Korea (NRF) funded by Ministry of Science and ICT (NRF-2017M3D1A1039379).

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 10:36

Chair: Kwang Seob Jeong (Korea University)

Physical-Organic Approach to Examine Structure-Rectification Relation through Investigation of Second-order Stark Effect

Soo jin Cho, Gyu Don Kong, Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

In principal, molecules exposed to an external electric field undergo distortion of electron orbit called the Stark effect. Understanding how the electronic function of molecular-scale electronic devices is related to the Stark effect is important. This presentation shows physical-organic studies to examine structure-property relationships in molecular-scale electronic devices. In particular, we focus on charge tunneling behaviors of large-area junctions formed with self-assembled monolayers comprising polycyclic aromatic hydrocarbon (PAH)-terminated *n*-alkanethiolates. No significant permanent dipole in the molecules allows us to investigate how the second-order Stark effect affect the performance of the PAH-based molecular diode. We demonstrate that the supramolecular structural change in a monolayer of the PAH-based molecular diode significantly influences the performance of device. The relation between the tilt angle of the active PAH terminal group relative to the direction of external electric field and the degree of the Stark shift and diode efficiency is quantitatively established.

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

Oral Presentation of Young Material Chemists

Room 405+406, THU 10:48

Chair: Kwang Seob Jeong (Korea University)

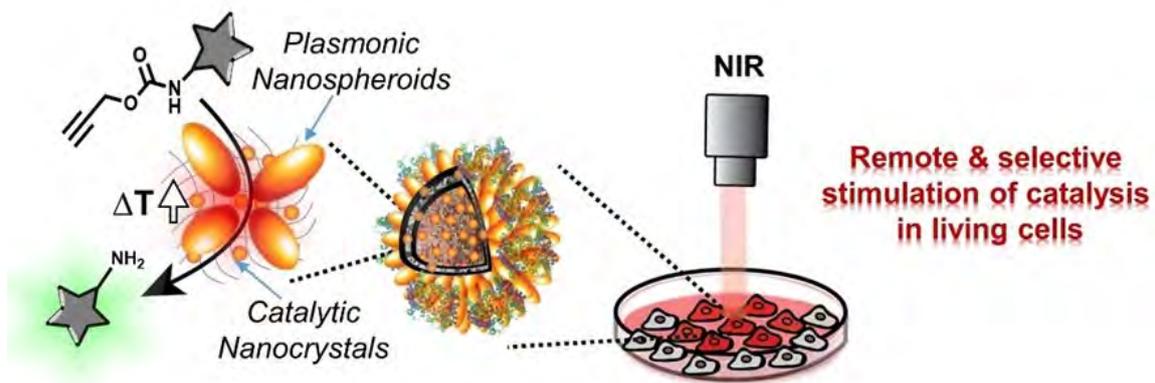
Remotely Operable and Highly Functional Plasmonically-Integrated Nanoreactors (PINERs) for NIR-Light-Induced Bioorthogonal Catalysis in Living Cells

Amit Kumar, In Su Lee^{1,*}

Chemistry, Pohang University of Science and Technology, Korea

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

Artificial nanoreactors that can facilitate catalysis in living systems on-demand with the aid of remotely operable and biocompatible energy-source, are needed to leverage the chemical diversity and expediency of chemical synthesis in biology and medicine. Here, we designed and synthesized plasmonically-integrated nanoreactors (PINERs) with highly tunable structure and NIR-light-induced synergistic function for efficiently promoting unnatural catalytic reactions inside living cells (Figure 1). We devised synthetic approach towards PINERs by investigating the crucial role of metal-tannin coordination polymer nanofilm — the pH-induced decomplexation-mediated phase-transition process — for growing arrays of Au-nanospheroid-units, constructing a plasmonic corona around the proximal and reactant-accessible silica-compartmentalized catalytic nanospace. Owing to the extensive plasmonic coupling effect, PINERs show strong and tunable optical absorption in NIR-range, ultrabright plasmonic light scattering, controllable thermoplasmonic effect and remarkable catalysis; and, upon internalization by cells, PINERs are highly biocompatible and demonstrate dark-field microscopy-based bioimaging features. Empowered with the synergy between plasmonic and catalytic effects and reactant/product transport, facilitated by the NIR-irradiation, PINERs can perform intracellular catalytic reactions with dramatically accelerated rates and efficiently synthesize chemically activated fluorescence-probes and anticancer drugs inside living cells. In future, PINERs can be advanced to the development of highly selective targeted theranostic platforms switchable in the response to the variety of designer biorthogonal catalytic reactions. Reference: Kumar, A. et al. ACS Catal., 2019, 9, 977–990.



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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:00

Chair: Jinho Chang (Hanyang University)

Utilization of photosynthetic organisms as photo-biocatalysts for solar energy conversion to electricity

Jinhwan Lee, Sunghyun Kim^{1,*}

Department of Biotechnology, Konkuk University, Korea

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Recently, there is a growing interest in solar energy conversion studies using photosynthetic organisms such as the thylakoid membranes (TMs), photosystem II (PS II), and photosystem I (PS I) as photo-biocatalysts. Here we present the novel bio-photoanode system based on the TMs to convert solar energy into electricity. To effectively form the TMs-based composite film on the electrode, the mesoporous graphite electrode capable of functioning as a filter was employed. TMs were introduced and electrically connected to the electrode by the indium tin oxide nanoparticles (ITOnp). The electron transfer between electrode and TMs was improved by the osmium redox polymer (Os-RP), and the enhanced photocurrent of 236 % compared to the TMs/ITOnp film was observed from the TMs/Os-RP/ITOnp film. Under one sun (100 mW cm⁻²) illumination, the maximum power density of photoelectrochemical cell (PEC) comprised of TMs/Os-RP/ITOnp film photoanode and Pt/C air-cathode is $121.8 \pm 9.5 \mu\text{W cm}^{-2}$ at the current density of $757.8 \pm 29.5 \mu\text{A cm}^{-2}$. In this study, the role of the TMs as photo-biocatalysts to convert solar energy was confirmed and the performance of the PEC was improved by effectively introducing TMs into the electrode.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:10

Chair: Jinho Chang (Hanyang University)

Composition-Dependent Electrocatalytic Activity of Cobalt Sulfides for Triiodide Reduction in Dye-Sensitized Solar Cells

Minsoo Kim, Jin Ho Bang*

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A new nanoarchitecture of cobalt sulfide (CoS_x) is designed by exploiting a Prussian blue analogue. Depending on the sulfidation temperatures, CoS_x materials with different compositions and morphologies are obtained. This investigation of the composition-dependent electrocatalytic activity of CoS_x for triiodide reduction reaction (IRR) reveals that sulfur-deficient CoS_x is more active than sulfur-rich CoS_x. When utilized in dye-sensitized solar cells (DSSCs), sulfur-deficient CoS_x with a hollow nanocube morphology outperforms platinum (Pt), showing great promise as a Pt alternative. This composition dependency on IRR is attributed to different surface characteristics and electrical properties that vary with CoS_x composition. This work highlights the importance of understanding the surface properties of sulfide-based electrocatalysts that are intimately dictated by their compositions as part of a new design principle for a highly active electrocatalyst.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:20

Chair: Jinho Chang (Hanyang University)

Rechargeable aluminium organic batteries

Dong-Joo Yoo, Jang Wook Choi*

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

Since aluminium is one of the most widely available elements in Earth's crust, developing rechargeable aluminium batteries offers an ideal opportunity to deliver cells with high energy-to-price ratios. Nevertheless, finding appropriate host electrodes for insertion of aluminium (complex) ions remains a fundamental challenge. Here, we demonstrate a strategy for designing active materials for rechargeable aluminium batteries. This strategy entails the use of redox-active triangular phenanthrenequinone-based macrocycles, which form layered superstructures resulting in the reversible insertion and extraction of a cationic aluminium complex. This architecture exhibits an outstanding electrochemical performance with a reversible capacity of 110 mA h g^{-1} along with a superior cyclability of up to 5,000 cycles. Furthermore, electrodes composed of these macrocycles blended with graphite flakes result in higher specific capacity, electronic conductivity and areal loading. These findings constitute a major advance in the design of rechargeable aluminium batteries and represent a good starting point for addressing affordable large-scale energy storage.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:30

Chair: Jinho Chang (Hanyang University)

The electronic structure of IrNiO_x electrocatalysts for oxygen evolution reaction in different pH electrolytic condition

Jaekyung Yi, Hyung-Suk Oh^{1,*}, Yun Jeong Hwang^{1,*}

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¹*Clean Energy Research Center, Korea Institute of Science and Technology, Korea*

Clean energy is attracting much attention as an alternative energy source because the energy supply and demand paradigm based on fossil fuels cause environmental pollution. In this respect, the hydrogen energy produced by the electrochemical water splitting has many advantages, such as high energy density, no self-discharge, no pollutants and so on. The water splitting consists of two electrochemical reactions: hydrogen evolution reaction (HER) in the cathode side and oxygen evolution reaction (OER) in the anode side. Most studies are focused on the oxygen electrode with high overpotential and this issue are addressed by controlling the electronic structure of the electrocatalysts. In general, the electronic structure of the electrocatalyst for OER can be interpreted with the coordination between d-orbitals (t_{2g} and e_g) of transition metal and oxygen. The issue of OER catalyst research is to change the electronic structure considering the electron occupancy and the density of state (DOS) of d-orbital in electrocatalysts, thereby reducing the overpotential and increasing the activity for OER. Herein, we synthesized IrNiO_x/C electrocatalyst for OER, which was improved OER activity by varying the pH electrolytic condition during the activation process. In order to prove the reason for the improved activity, we analyzed the electronic structure of IrNiO_x/C with different pH condition using in-situ XAFS. The physical properties were also analyzed using IL-TEM, XPS, XRD, and ICP-OES.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:40

Chair: Jinho Chang (Hanyang University)

Electrochemical Detection and Electrolysis of Single Nanosized Water Droplet Collisions in Organic Solution

Jungeun Lee, Byung-Kwon Kim*

Department of Chemistry, Sookmyung Women's University, Korea

Direct electrolysis and detection of single nanosized water emulsion droplets in organic solution using the electrochemical stochastic collision technique on an ultramicroelectrode (UME) was studied. Emulsions, which are a special type of mixture of two or more immiscible liquids, has attracted extensive attention not only in scientific research but also in industries such as cosmetics, food, pharmacy, construction, and petroleum. Despite their outstanding advantages, some water/oil (W/O) emulsions can cause unexpected results, which significantly affect the quality of products, especially in the petroleum industry. Consequently, the detection of the presence and property of W/O emulsion is necessary to evaluate the quality of products. In this experiment, the detection system for water droplets does not require any kind of redox species in an organic solvent, only water molecules in the water droplets were considered. When water droplets collided with the UME surface, anodic current spikes were observed in the chronoamperometry, resulting from the electrolysis of water molecules in the water droplets. From the collision frequency and integrated current spike, concentrations and size distributions of water droplets in an organic solvent can be determined.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 09:50

Chair: Jinho Chang (Hanyang University)

Unraveling the Controversy over the Catalytic Reaction Mechanism using a New Theoretical Methodology: One Probe and Non- Equilibrium Surface Green's Function

Chiho Lee, Sang Uck Lee*

Department of Bio-Nano Engineering, Hanyang University, Korea

We shed light on the longstanding controversial issues on the iodine reduction reaction (IRR) mechanism using a new proposed methodology called “One Probe and Non-equilibrium Surface Green's function (OPNS)”. The OPNS approach completely alleviates the limitations of traditional slab approach for the electrocatalytic reactions by coupling the surface to an infinite reservoir of electrons at a fixed chemical potential and implements an external electric field environment through a semi-infinite one probe model. With aid of OPNS and in-depth structural analysis under the external electric field, we re-evaluated the previously proposed IRR mechanisms on the Pt(111) surface, consecutive and concerted mechanisms. Our results reveal that the configurational preference of approaching I₂ molecules depending on the external electric field governs the IRR mechanism. Under the reductive potential, I₂ molecules prefer vertical (I₂V) configuration rather than parallel (I₂P) configuration, which leads to the consecutive mechanism where I atoms are sequentially reduced due to asymmetric charge accumulation on a single I atom to be initially desorbed. Consequently, we can clarify that the IRR follows the consecutive mechanism and we believe that the new OPNS method and the proposed onset threshold electric field for reduction as an effective descriptor of catalytic activity evaluation can inspire the study of electrocatalytic reactions for various catalysts.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 10:00

Chair: Jinho Chang (Hanyang University)

A stand-alone electrocatalytic system combined arsenic oxidation and CO₂ reduction

Wonjung Choi, Hyunwoong Park*

School of Energy Engineering, Kyungpook National University, Korea

A stand-alone simultaneous drive system combined electrocatalytic arsenite oxidation and CO₂ reduction to formate with nearly 100% Faradaic efficiencies in both reactions was first implemented. The conversion of CO₂ to formate in bicarbonate solution at the circum-neutral pH was carried out on the Bi electrode synthesized onto Ti plate by electrodeposition method, and this electrocatalytic CO₂ reduction reactions was combined with arsenic oxidation which performed on commercial TiO₂ nanoparticle electrocatalyst (n-TEC). In half-reaction experiments performed prior to combination, As(III) oxidation and formate production were respectively optimized, and the production of As(V) and formate were enhanced by adding chloride in electrolyte. In the combination system, in order to prevent undesired re-oxidation and re-reduction in the counter electrode, both electrodes were divided by a proton-exchange membrane and different anode/cathode area ratios were applied to obtain two optimal operating conditions. It was confirmed that the simultaneous system combining each half-reactions was successfully combined without deteriorating the performance of any electrocatalytic reaction. The simultaneous system was finally designed as a stand-alone system that does not require external grid by coupling with the PV panels. This research was supported by the Basic Science Research Program (2016R1A2B4007366 and 2018R1A6A1A03024962) through the National Research Foundation, Korea.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 10:10

Chair: Jinho Chang (Hanyang University)

A Quantitative Method to Measure Corrosion Current on Zinc Metal Electrodes

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Researches on zinc metal-based batteries have attracted considerable attention as a candidate for post lithium-ion batteries. Zinc is one of few metal anodes that are compatible in aqueous as well as non-aqueous electrolytes, providing a large theoretical capacity of 820 mAh g^{-1} . However, in aqueous electrolytes, zinc metal anode suffers from hydrogen evolution reaction (HER), by which zinc is irreversibly consumed or corroded continually. Exact estimation of the corrosion current has been a challenge in the development of Zn-based batteries. Measurement of corrosion current by conventional Tafel analysis meets serious problems because the cathodic current reflects deposition of Zn metal as well as HER, inhibiting exact measurement of corrosion current. Herein, we developed "Depo-Rest-Diss" method to quantify the corrosion current without such interference from the deposition of Zn. The "Depo-Rest-Diss" method was successfully applied to the quantification of corrosion current in aqueous electrolytes with various pH and concentration. The "Depo-Rest-Diss" method and electrochemical impedance spectroscopy confirmed that saturated ZnSO_4 (ca. 3.2 M) + 0.075 M Li_2SO_4 delivers the lowest corrosion current compared to the other electrolytes probably because the activity of water in such concentrated electrolyte is low enough to suppress the kinetics of HER. Thus developed "Depo-Rest-Diss" method can be generally applied to determine the corrosion current on various metal electrodes.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 10:20

Chair: Jinho Chang (Hanyang University)

Electrochemistry of Rationally Designed Metal Nanoclusters in Atomic Precision.

Kyuju Kwak, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

For the past few years, atomically precise metal nanoclusters containing a few to a few hundreds of metal atoms have been the focus of recent investigations because of their novel physicochemical properties with high stability. This presentation focus on recent progress made in the electrochemistry of the atomically precise metal nanoclusters and their applications in electrocatalysis. A sizable opening of HOMO-LUMO gap observed for Au₂₅ in voltammograms gradually decreases with increasing nanocluster size, which is in line with the change in the optical gap. In addition to the size effects, the difference in chemical composition is also sensitively detected by voltammetry. The HOMO-LUMO gaps of Pt- and Pd-doped Au₂₅ determined by voltammetry were drastically decreased indicating that their electronic structures were significantly altered upon doping of the foreign metal. Furthermore, heteroatom doping has been a powerful strategy to tune the electronic properties of metal nanoclusters at the atomic level, which offers great potential for achieving high activity in their electrocatalytic applications. The Pt-doped Au₂₅ nanocluster shows the excellent electrocatalytic activity toward hydrogen evolution reaction. This can be ascribed to the positive shift of the reduction potential that matches well with the reduction potential of proton and its thermodynamically neutral binding energy for proton adsorption. Consequently, the atomically controlled metal nanoclusters will enable us to systematically optimize the electrochemical properties suitable for electrocatalysis, thus providing a powerful platform for the discovery of finely tuned nanocatalysts.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 407+408, THU 10:30

Chair: Jinho Chang (Hanyang University)

Degradation Mechanisms in Lithium-Ion Batteries with Layered Transition Metal Oxide Based Cathode Active Materials

A.T.S. Freiberg, H.A. Gasteiger^{*}, R. Jung, M. Metzger, S. Solchenbach, B. Strehle, T. Teufl, J. Wandt

Technical Electrochemistry, Dept. of Chemistry and Catalysis Research Center, Germany

Promising cathode active materials (CAMs) to increase the energy density of lithium ion batteries are nickel-rich NCM ($\text{LiNi}_x\text{Co}_y\text{Mn}_z\text{O}_2$ with $x+y+z=1$) and overlithiated so-called HE NCM ($\text{Li}_{1+x}\text{M}_{1-x}\text{O}_2$; with $\text{M}=\text{Ni, Co, Mn}$)^{1,2}. However, at high states-of-charge (SOC), molecular oxygen is released from the surface of these materials, not only leading to a growth of the cathode impedance, but also to enhanced electrolyte oxidation^{3,4}. Based on these observations, we suggested that the overall oxidation of the electrolyte can be distinguished into a chemical oxidation mechanism triggered by the release of active oxygen at high SOC and into a purely electrochemical oxidation mechanism initiating at high potentials⁵.

Using on-line electrochemical mass spectrometry (OEMS)³⁻⁵ and operando emission spectroscopy, we will provide evidence that the chemical electrolyte oxidation mechanism is triggered by the release of singlet oxygen from NCM and HE NCM surfaces at high SOC. It will be discussed how the reaction of singlet oxygen with the electrolyte solvents can result in the formation of protic species⁶, leading to transition metal dissolution from the CAMs⁷. As dissolved transition metals will deposit on the lithium-ion battery anode, the effect of transition metals on the stability of the graphite SEI will also be discussed⁸.

References:

1. D. Andre, S.-J. Kim, P. Lamp, S.F. Lux, F. Maglia, O. Paschos, B. Stiaszny, *J. Mater. Chem. A* 3 (2015), 6709.
2. K.G. Gallagher, S. Goebel, T. Greszler, M. Mathias, W. Oelerich, D. Eroglu, V. Srinivasan, *Energy Environ. Sci.* 7 (2014) 1555.
3. B. Strehle, K. Kleiner, R. Jung, F. Chesneau, M. Mendez, H.A. Gasteiger, M. Piana, *J. Electrochem. Soc.*

164 (2017) A400.

4. R. Jung, M. Metzger, F. Maglia, C. Stinner, H.A. Gasteiger, *J. Electrochem. Soc.* 164 (2017) A1361.

5. R. Jung, M. Metzger, F. Maglia, C. Stinner, H.A. Gasteiger, *J. Phys. Chem. Lett.* 8 (2017) 4820.

6. A.T.S. Freiberg, M.K. Roos, J. Wandt, R. de Vivie-Riedle, H.A. Gasteiger, *J. Phys. Chem. A* 122 (2018) 8828.

7. J. Wandt, A.T.S. Freiberg, R. Thomas, Y. Gorlin, A. Siebel, R. Jung, H.A. Gasteiger, M. Tromp, *J. Mater. Chem. A* 4 (2016) 18300.

8. S. Solchenbach, G. Hong, A.T.S. Freiberg, R. Jung, H.A. Gasteiger, *J. Electrochem. Soc.* 165 (2018) A3304.



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

New Trends in Chemistry Education

Room 204, THU 09:00

Chair: Aeran Choi (Ewha Womans University)

Analysis of experiments related to electrolysis of aqueous solution in chemistry textbooks of secondary schools

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¹Chemistry, Sejong Academy of Science and Art, Korea

In this study, we compared the content of textbooks of 2009 revised curriculum with the contents of textbooks of 2015 revised curriculum in order to check whether there is a change in "development and use of model" which is emphasized in 2015 revised curriculum. To do this, we analyzed 4 kinds of chemistry I textbooks and 4 kinds of chemistry II textbooks in the revised 2009 curriculum and compared them with 7 kinds of chemistry I textbooks and 5 kinds of chemistry II textbooks in 2015 revised curriculum. The scope of the analysis was focused on only the explanations and experiments presented in the textbooks. In order to compare the contents of electrolyte, we analyzed contents of 9 kinds of middle school science textbooks of 2009 revision curriculum and 3 kinds of middle school science textbooks of 2015 revision curriculum. As a result of the analysis, the same experiment was explained by different models according to grade and unit, and all explanations were limited to a single model. Also, the tendency to limit the use of electrolytes with experimental results, which may not be consistent with the model, is more pronounced in the 2015 revised curriculum than in the 2009 revised curriculum. These results suggest that emphasis should be need the "development and use of models" in textbook experiments and explanations of the 2015 revised curriculum.

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

New Trends in Chemistry Education

Room 204, THU 09:20

Chair: Aeran Choi (Ewha Womans University)

Development of an Assessment Method for Scientific Creativity of Scientific Products Base on Analogical Thinking and Its Application

Hunsik Kang

Elementary Gifted Education, Seoul National University of Education, Korea

This study developed and applied an assessment method for scientific creativity of scientific products (i.e., scientific humor) base on analogical thinking. The creativity of science humor was divided into five categories: fluency, flexibility, usability, originality, and total creativity. Science humor fluency, which is related to how much science humor is produced in a limited time, was evaluated using the number of students' scientific humor. As science humor flexibility is related to how diverse the thinking is, it was evaluated using the classification criteria according to the 'form' of the analysis criteria for scientific humor of the previous research (Lee & Kang, 2018). In other words, the flexibility was assessed separately for the flexibility according to 'generation form' and the flexibility according to 'description form', and the sum of the two scores was calculated as the scientific humor flexibility score (10 out of 10). Science humor usability was evaluated using the mean of the usability scores evaluated by one's self and two or three members of a team about one science humor that students selected as the most new and useful among their scientific humor. Two times the corresponding average was calculated by the student's science humor usability score (10 out of 10). Scientific humor originality was calculated by using creativity factor in the scientific creativity evaluation formula of Lim (2014) to investigate how students make novel types of scientific humor. In this study, 'n' was the number of ideas belonging to a specific type of 'generation form', and N was the total number of ideas. And the 'generation form' originality score and 'description form' originality score were calculated for each science humor and the average of two originality scores was calculated as scientific humor originality score (10 out of 10). Based on these criteria, each student's scientific humor was analyzed and the highest originality score was calculated as the student's scientific humor originality score. The total scientific humor creativity was calculated by using the scientific creativity evaluation formula of Lim (2014) based on originality and fluency. In this formula, the former was the originality factor and the latter was the usability factor, so the science humor creativity score and the

usability score were used to calculate the science humor creativity score. This study introduced the application of the scientific humor creativity evaluation method. This kind of scientific creativity evaluation method can provide useful implications for quantitative evaluation and effectiveness verification methods of scientific creativity in scientific products (i.e., scientific analogies, poems, humors etc.) base on analogical thinking.



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

New Trends in Chemistry Education

Room 204, THU 09:50

Chair: Aeran Choi (Ewha Womans University)

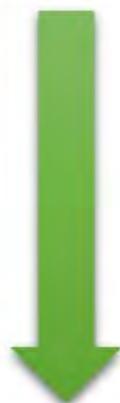
A Hands-on Experiment to Verify Consistency from Bulk Density to Atomic and Ionic Radii with Lumps of Metals and Ionic Compounds

Seong Kyun Kim^{*}, Seounghey Paik^{1,*}

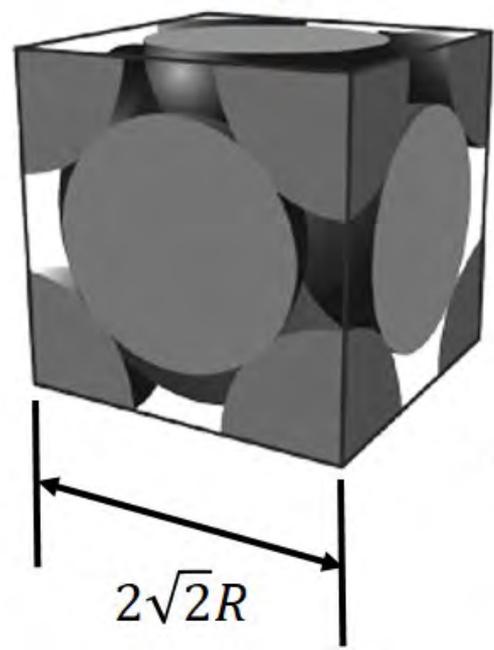
School of Undergraduate Studies, Daegu Gyeongbuk Institute of Science & Technology, Korea

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

A hands-on experiment to obtain atomic and ionic radii with lumps of metal and ionic compounds is reported here. The experiment is performed with industrial-grade typical metals (iron, copper, aluminum, and lead) and single-crystal lumps of ionic compounds (sodium chloride, potassium chloride, and potassium bromide). Students measure the dimension of the given lumps with Vernier calipers and weigh them with a precision balance. After measuring the dimension and mass of the given lumps, students can calculate the atomic and ionic radius of each corresponding atom and ion with the obtained density values and information about the lattice structures. The obtained values of the metal atomic radii and the ionic radii of ionic compounds are very close to values in the literature. After this activity, the students came to appreciate that atomic radii, as typical sub-microscopic and symbolic representations, are actually existing features and not an abstract concept. The experiment reported here is suitable for a first-year undergraduate general chemistry class as well as an introductory class at the high school level.



hands-on measurement



Lattice Structure?
Atomic Radii?

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

New Trends in Chemistry Education

Room 204, THU 10:10

Chair: Aeran Choi (Ewha Womans University)

Chemistry Experiment Class in High School

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

How can high school students study chemistry fun? Chemistry can be fun to learn through chemistry experimental activities. However, The chemistry contents in high school are not easy learned through chemistry experimental activities. The reason is in the limits of chemical experiment environment and the contents of chemistry experiment class. In high school chemistry experiment subject faces to many limitations, not only due to limitations on the experimental space or the experimental class time, but also due to the various risks associated with the experimental activities. It also requires to develop the contents of chemical experiment class in high school. Despite these limitations, students should be encouraged to learn chemistry through experimental activities in high school. we try to educate through not only experimental activities by introducing project-oriented experimental activity class in fundamental organic chemistry but also General Chemistry Lab 1 and General chemistry Lab 2 which are accelerated deepening courses at Korea Science Academy of KAIST. In this presentation, we discuss how to teach chemistry through experimental activities in high school.

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

Student Oral Presentation

Room 203, THU 09:00

Chair: Kiyoung Lee (Kyungpook National University)

The Effects of Metal-doping and Surface Modification on Hydrogen Production Activity of Metal Nanoclusters

Woojun Choi, Kyuju Kwak, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Identification of an efficient hydrogen evolution reaction (HER) electrocatalyst is one of the challenging fields to replace fossil fuel. Although many efforts to develop an active HER catalysts, it is still uneasy to answer what is the main factor that influence on HER activities. Among many researches, two factors are commonly accepted that one is thermoneutral binding step with H^+ ($\Delta G_H = \sim 0$ eV) on solid metal catalysts and another is proton shuttling effect of secondary coordinated ligand of molecular catalysts. Ligand protected Au nanoclusters that have both metallic and molecular-like properties exhibit distinctive electrochemical and HER features. The HER activities of Au nanoclusters could be improved by doping of foreign metal and surface modification. In this presentation, we report electronic structures and catalytic properties of $Au_{25}(SR)_{18}$ and bimetallic $PtAu_{24}(SR)_{18}$ 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 Pt ($PtAu_{24}(C_6S)_{18}$, $33.4 s^{-1}$) and calculated ΔG_H by density functional theory supported the enhanced HER activities of doped nanoclusters. The TOF of Pt-doped nanocluster could further increase by introducing proton shuttling sulfonate ligands reached to $100 s^{-1}$ at -0.6 V.

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

Student Oral Presentation

Room 203, THU 09:15

Chair: Kiyoung Lee (Kyungpook National University)

Removal of aqueous Hg(II) using indium-modified bimetallic iron particles

Qasim Ghulam Hussain, Seunghee Han^{1,*}

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Zero-valent iron (ZVI) one of the most capable remediation technologies for organic and inorganic pollutants in water associated with its low cost and high reactivity. In order to maximize the reactivity and durability of microscale ZVI, the surface of ZVI was impregnated with Ni, Cu, and In, and the removal efficiency was batch-tested for 60 minutes with 250 nM of aqueous Hg(II) under pH 7. Among these metals, In-doped ZVI (In-ZVI) showed the highest Hg(II) removal efficiency of 99% along with the highest concentration of Hg(0) in the headspace, while the Hg(II) removal efficiency ranged from 3 to 15% with Ni and Cu modification. The sorption of Hg was better explained by Freundlich model than Langmuir model, suggesting that it may take place in a multilayer adsorption manner with irregular energy distributions. Furthermore, there was no significant decrease in the Hg(II) removal efficiency after seven successive runs, while it was largely decreased at the fourth cycle without In doping. The various control test results demonstrated that simple Hg sorption on ferric oxides or Hg reduction by In(0) or Fe(II) on ferric layer cannot support high removal efficiency of In-ZVI particles. Overall results suggest that a galvanic cell formed between In(0) oxidation and Fe(III) reduction on the surface of ZVI leads to the generation of atomic hydrogen, and it highly increased the Hg(II) reduction rate due to enhanced electronic interactions between Fe, In, and Hg.

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

Student Oral Presentation

Room 203, THU 09:30

Chair: Kiyoung Lee (Kyungpook National University)

Sb speciation and distribution in soils near a Sb refining factory and a shooting range

Soo-Chan Park, Man Jae Kwon^{1,*}

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¹*Korea University, Korea*

A large quantity of Sb, the 9th-most mined metal worldwide, and Sb-contained compounds have been released into the surface and subsurface environments. Sources of Sb release include abrasion from brake linings, use as flame retardants, plastic production, mining and shooting activities. Though the ecotoxicity of Sb is not well known, Sb(III) compounds are generally considered to be more toxic and mobile than Sb(V), similar to that of As. Therefore, distribution, speciation, toxicity and bioavailability in various environmental compartments are some of main interests related to Sb and important for human and ecosystem health. In this study, the Sb distribution and biogeochemical characteristics of contaminated soils in the vicinity of Sb refining factory (n=22), antimony waste landfill site (n=14) and shooting range (n=12) in South Korea were investigated. Soil samples adjacent to Sb refining factory (220 ~ 4918 mg/kg) and antimony waste landfill site (25.65 ~ 12432.5 mg/kg) generally represented higher Sb concentrations than those in the shooting range (15 ~ 39.8 mg/kg). However, the samples from the shooting range showed multiple contamination with Pb and other heavy metals. Except the landfill site, the concentrations of Sb were also depth dependent and markedly decreased with depth. Microbial population determined by the most probable number at each site showed relatively low cell number ($10^4 \sim 10^5$) in the sites with high Sb concentrations than uncontaminated soils ($10^6 \sim 10^7$). 16S rDNA analysis will be used to characterize the microbial community structures in each site which will be discussed in the relation to the content and speciation of Sb in soils determined by X-ray Absorption Fine Structure (XAFS) and sequential extraction analysis.

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

Student Oral Presentation

Room 203, THU 09:45

Chair: Kiyoung Lee (Kyungpook National University)

Mineral precipitates and microbial community compositions in groundwater from inside waste disposal site

Bak Noon Ham, Man Jae Kwon^{1,*}

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Constructing deep underground waste storage sites can cause dramatic changes in groundwater quality as well as groundwater flow, and these changes subsequently influence subsurface microbial activities and community compositions. To understand how the underground construction influences the subsurface environments, we investigated geochemical variations, major mineral precipitates and microbial community compositions at different locations of the waste disposal sites (WS1~6) in the vicinity of coastal region in South Korea. Groundwater drained from WS1, WS2, WS3, and WS5 was Ca-Cl-type with relatively high Total Dissolved Solids (TDS), while that from WS4 and WS6 was Ca-Na-HCO₃ type. Br/Cl and $\delta D/\delta^{18}O$ ratios showed that the groundwaters of WS1(15%), 3(2%) and 5(5%) were affected by seawater. Various sulfate reducing bacteria were identified with relatively high sulfate due to the saltwater mixing at these locations. High abundance of *Geobacter* and *Gallionella* at WS3 indicated that they contributed to a high Fe concentration in groundwater and the formation of various iron minerals (i.e., Fe(OH)₃, α -FeOOH, FeCO₃, green rust). WS5 and WS6 showed extremely high pH (>10) and very high abundance of *Hydrogenophaga* previously discovered in alkaline groundwater (pH>10) or sediment as alkali-tolerant bacteria. Thermoanaerobacterales, halophilic and alkalithermophilic bacteria, was also predominant at WS5 and WS6. The results showed that groundwater drained from inside the waste disposal site was distinct at each location and strongly influenced by localized geochemical conditions (i.e., high alkalinity, salinity and oxidation). These groundwaters further impact mineral precipitates and microbial community structure.

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

Student Oral Presentation

Room 203, THU 10:00

Chair: Kiyoung Lee (Kyungpook National University)

Red mud induced photocatalysis in the presence of peroxides

Joohyun Kim, Sungjun Bae*

Department of Environmental Engineering, Konkuk University, Korea

Red mud (RM) is a solid waste from Bayer process, which can cause severe environmental problems. To reuse the RM, we developed a novel photocatalysis system (RM + peroxides (i.e. hydrogen peroxide (H_2O_2), peroxymonosulfate (PMS) and persulfate (PS)) for wastewater treatment under visible light irradiation. Acid orange 7 (AO7) was selected as a target pollutant in this study. The amount of peroxide consumed after the complete decolorization was ordered as follows: $\text{PS} < \text{PMS} < \text{H}_2\text{O}_2$, indicating the highest efficiency of PS for the AO7 decolorization. In order to investigate the photocatalysis mechanism, we prepared different metal oxide (M_xO_y) composites and Fe_2O_3 was found to be a main player for the degradation of AO7 by forming AO7- Fe^{3+} complex. Compared to pure Fe_2O_3 , $\text{Fe}_2\text{O}_3\text{-Na}_2\text{O}$ composite showed enhancement in decolorization rate due probably to the peroxide activation by continuous extraction of OH^- anion, whereas $\text{Fe}_2\text{O}_3\text{-Al}_2\text{O}_3$ and $\text{Fe}_2\text{O}_3\text{-SiO}_2$ composites showed a remarkable inhibition effect on decolorization. To investigate the main reactive radical species, we used various radical scavengers (i.e. 2-propanol, phenol, p-benzoquinone, sodium azide and N_2 purging) and found out that superoxide radical ($\text{O}_2^{\cdot -}$) or hydroperoxy radical (HO_2^{\cdot}) were the main radical species as an initiator, resulting in the activation of peroxides for AO7 decolorization. The results of this study revealed that red mud can be successfully utilized for AO7 decolorization as a catalyst without any pre-treatment or modification. **Keywords:** Red mud, Acid Orange 7, Visible light, Decolorization, Persulfate

Acknowledgments This work is supported by the National Research Foundation of Korea (project no. 2016R1D1A1B03930142 and 2019R1C1C1003316).

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

Student Oral Presentation

Room 203, THU 10:15

Chair: Kiyoung Lee (Kyungpook National University)

Effect of natural organic matter on TiO₂ photocatalysis under visible light illumination via ligand-to-metal charge transfer (LMCT)

Hyeonyeong Park, Wooyul Kim^{1,*}, EunJu Kim*

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

¹*Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea*

The severe interference of natural organic matter (NOM) during TiO₂ photocatalysis makes its practical application difficult although TiO₂ photocatalysis has been extensively studied in advanced oxidation process for water treatment system. Revealing the interaction between NOM and TiO₂ is important to prevent inhibitory effect of NOM and enhance the photocatalytic efficiency of TiO₂. However, most studies have focused on the interaction NOM with TiO₂ under UV light conditions and relatively little is known about the role of NOM in TiO₂ photocatalysis under visible light conditions. Here, the role of humic acid (HA) in the photocatalytic activity of TiO₂ under visible light condition was systematically investigated. The HA-coated TiO₂ (HA/TiO₂) has a continuous absorption in the visible region extending to 800 nm that is not observed in HA or TiO₂ only. It is assigned to the ligand-to-metal charge transfer (LMCT) transition ($\text{HA} + \text{TiIV} \rightarrow \text{HA}^+ + \text{TiIII}$). Some substrates (4-chlorophenol and Cr(IV)) were clearly reduced in the presence of HA/TiO₂ under visible irradiation while dichloroacetate was not decomposed at all. Such a substrate-specific property was related with reactive oxygen species (ROS) generated in HA/TiO₂ under visible illumination. The details for ROS produced will be presented.

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

Student Oral Presentation

Room 203, THU 10:30

Chair: Kiyoung Lee (Kyungpook National University)

Phase dependent OH radical Generation Mechanism: Anatase vs. Rutile TiO₂

Ji Young Hwang, Wooyul Kim^{1,*}

Department of Chemical and Biological Engineering, Sookmyung women's university, Korea

¹*Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea*

TiO₂ as a photocatalyst is a widely investigated for very diverse applications because it is eco-friendly and inexpensive. Although intensive research has been reported, the complete understanding of photocatalytic phenomenon and mechanisms of mobile hydroxyl radical generation is still far away. In this study, selective generation of mobile hydroxyl radicals on anatase of TiO₂ was confirmed using tetramethylammonium (TMA) in acidic condition, but its decomposition was negligible on the rutile phase. The pH-dependent electrostatic interactions cause the surface trapped holes to participate in the oxidation of TMA by adsorbing TMA to anatase and rutile in base condition by changing the decomposition behavior of TMA. Thus, the trend selectively distinguishes a surface trapping holes and a mobile hydroxy radical derived from photocatalysis. The direct evidence gathered from various spectroscopic and photocatalytic TMA decomposition results will help to reveal the controversial mechanism mediating hydroxyl radicals, raised in diverse advanced oxidation processes.

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

Student Oral Presentation

Room 203, THU 10:45

Chair: Kiyoung Lee (Kyungpook National University)

Mercury Isotope Investigation of Sources and Transport of Mercury in a Creek Impacted by Multiple Anthropogenic Activities

Saebom Jung, Sae Yun Kwon*

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

Measurements of natural abundances of mercury stable isotopes in environmental samples have enhanced the understanding of mercury sources and biogeochemical processes in natural environments (e.g. Blum et al. 2014). The mixing of multiple mercury sources and two types of fractionation pathways known as mass-dependent (MDF, reported as $\delta^{202}\text{Hg}$) and mass-independent fractionation (MIF; reported as $\Delta^{199}\text{Hg}$) have provided insight to environmentally relevant processes governing changes in mercury isotope ratios of environmental samples. Thus far, the application of mercury isotope ratios has been particularly active in the discipline of environmental forensic for characterizing the environmental impacts of known point sources of mercury and their distribution. In our study, we used mercury stable isotope analysis as a tool for characterizing unknown point sources of mercury in the contaminated sites of Gumu Creek, which flows along the industrial complex in the city of Pohang. Total mercury (THg) concentrations and mercury stable isotope ratios ($\delta^{202}\text{Hg}$ and $\Delta^{199}\text{Hg}$) were measured from the aquatic environment of the mercury-contaminated site in Pohang. By analyzing mercury stable isotopic compositions and by using a binary mixing model, we identified two potential mercury sources. Here, we demonstrate how mercury stable isotope analysis can be used to identify sources of mercury in the Gumu Creek, Pohang and their distribution in the environment. To our knowledge, this is the first attempt to use mercury stable isotope ratios as a major tool for identifying unknown point sources of mercury in the contaminated sites in South Korea.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Comparison of water absorption between PSMA ionomer and PSITA ionomer

Joon-Seop Kim^{*}, Seokyoung Park¹, Yoon Gwan Jeong¹

Department of Polymer Science and Engineering, Chosun University, Korea

¹Department of Polymer Chemistry Engineering, Chosun University, Korea

In this work, the water absorption behavior of PSMA ionomer and PSITA ionomer was compared. In both ionomer systems, the water uptake increased with increasing ion concentration. When the ionic concentrations of the two ionomers were less than 15 mol%, the water uptake increased by about 1 wt%/(mol% of ion content). On the other hand, high ion content PSMA ionomers (> 15 mol%) showed a rapid increase of water uptake by about 2.5 wt%/(mol% of ion content). This implied that in the carboxylated polystyrene ionomers a remarkable change in physical properties took place at the ion concentration of 15 mol%. Interestingly enough, "15 mol%" coincided with the ion content, at which the ion-containing polymers were classified into either ionomers (< 15 mol%) or polyelectrolytes (>15 mol%).

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

Polymer Chemistry

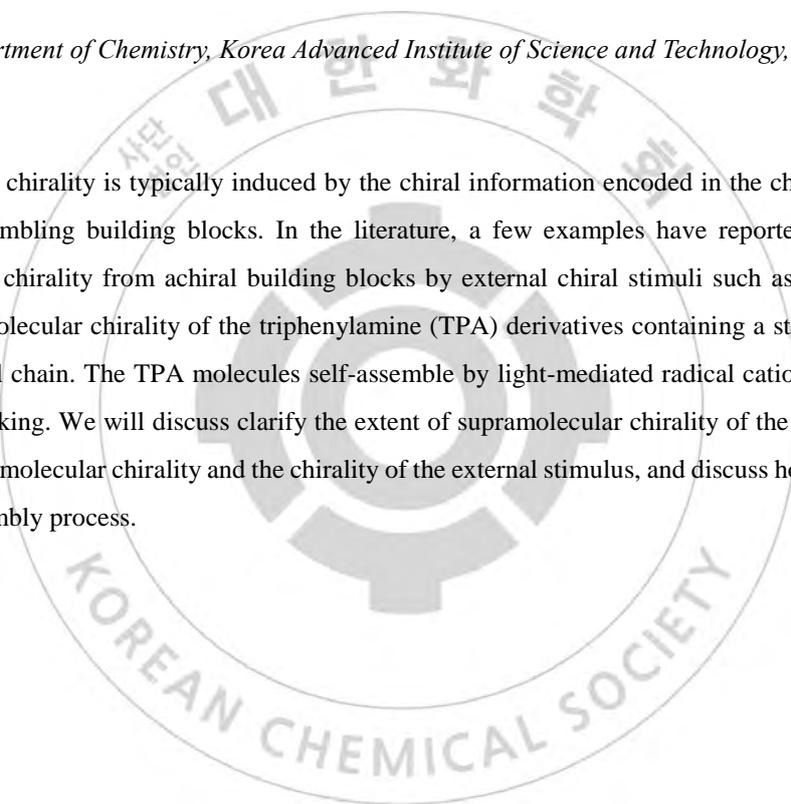
Exhibition Hall 2, FRI 11:00~12:30

Intrinsic and Extrinsic Encoding of Supramolecular Chirality

Jun Su Kang, Myungeun Seo*

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

Supramolecular chirality is typically induced by the chiral information encoded in the chemical structure of the self-assembling building blocks. In the literature, a few examples have reported emergence of supramolecular chirality from achiral building blocks by external chiral stimuli such as light. Here, we explore supramolecular chirality of the triphenylamine (TPA) derivatives containing a stereogenic center in the side alkyl chain. The TPA molecules self-assemble by light-mediated radical cation formation and subsequent stacking. We will discuss clarify the extent of supramolecular chirality of the TPA aggregates driven from the molecular chirality and the chirality of the external stimulus, and discuss how they compete in the self-assembly process.



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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Extremely Active MAO Free Chromium Catalyst For Ethylene Tetramerization

Hee soo Park^{*}, Bun Yeoul Lee^{1,*}, Taejin Kim

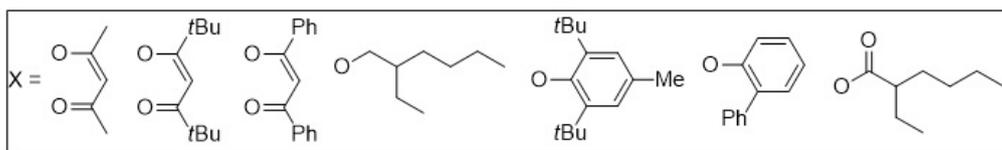
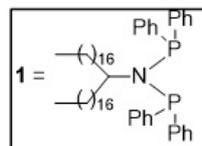
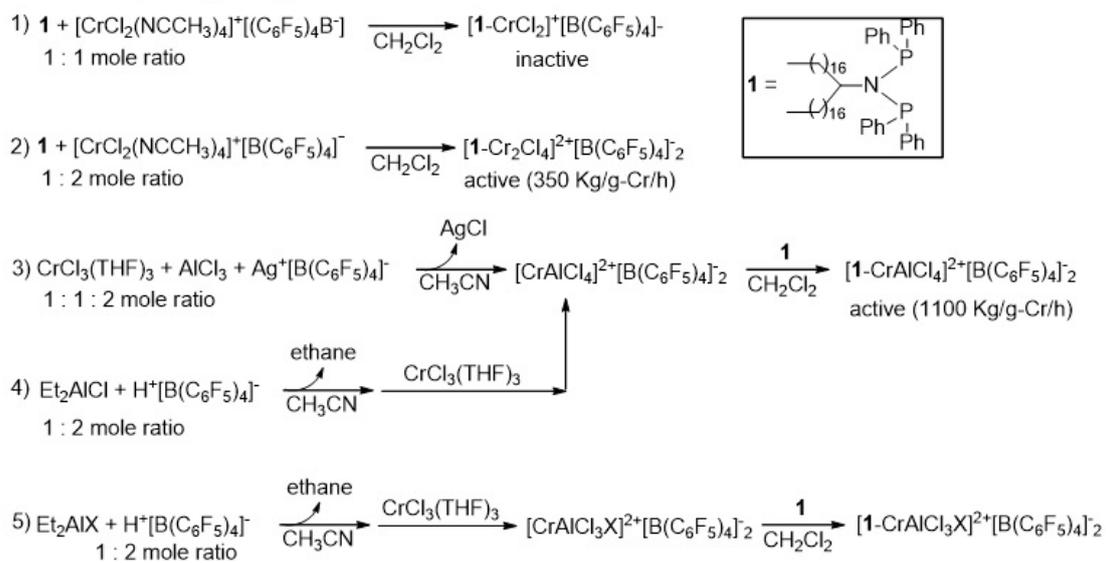
Molecular Science and Technology, Ajou University, Korea

¹*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. Therefore, 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 ($[(i\text{PrN}(\text{PPh}_2)_2)_2\text{CrCl}_2(\text{CH}_3\text{CN})_2]+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ or $[[\text{CH}_3(\text{CH}_2)_{16}]_2\text{CHN}(\text{PPh}_2)_2)_2\text{CrCl}_2(\text{CH}_3\text{CN})_2]+[\text{B}(\text{C}_6\text{F}_5)_4]^-$). 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 clearly 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 satisfactory. 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. Conclusionally, $[(\text{PNP})\text{CrCl}_2(\text{CH}_3\text{CN})_2]+[\text{B}(\text{C}_6\text{F}_5)_4]^-$

/Et3Al exhibited considerably higher activity than that of a previously reported system consist of [Ph3C]+[B(C6F5)4]-, i.e., 1/CrCl3(THF)3/[Ph3C]+[B(C6F5)4]-/Et3Al.

Scheme 1 (or Figure 1).



Poster Presentation : POLY.P-4

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Treatment of Peroxide Mediated C(sp³)-C(sp³) Coupling reaction: Synthesis of ABA-Type Olefin Triblock Copolymers

Hyunju Lee, Junwon Baek¹, Bun Yeoul Lee^{2,*}

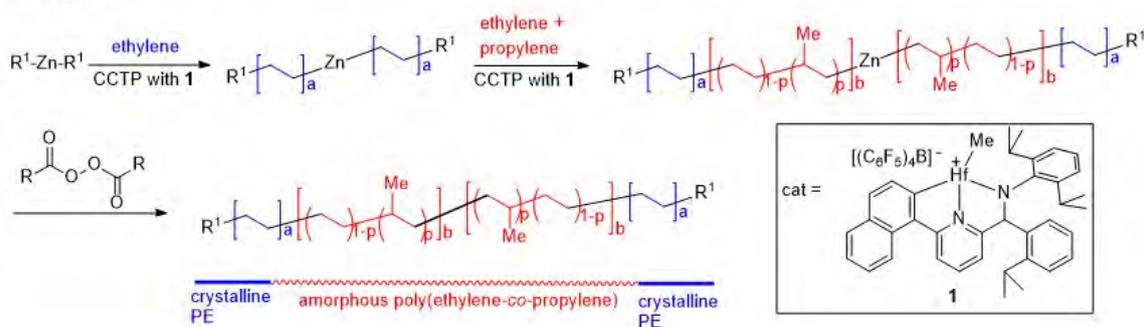
Department of molecular science and technology, Ajou University, Korea

¹*Ajou University, Korea*

²*Department of Molecular Science and Technology, Ajou University, Korea*

In this study, a useful and simple synthesis method of ABA-type olefin triblock copolymers, (e.g., PE-b-poly(ethylene-co-propylene)-b-PE) has been explained. 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)O-OC(O)(CH₂)₁₀CH₃) resulted in a C(sp³)-C(sp³) coupling reaction between the two diblock chains bound on the zinc site and an ABA-type olefin triblock copolymer, PE-b-poly(ethylene-co-propylene)-b-PE, was formed. When lauroyl peroxide was treated, the number average molecular weight increased by 1.5–1.7 times. The occurrence of the coupling reaction was confirmed using a model compound, Dioctylzinc as CTA(Chain Transfer Agent) for CCTP. 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.

Scheme 1



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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Self-assembly of Chiral Amphiphilic Random Copolymer in Aqueous Media

Minjoong Shin, Myungeun Seo*

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

Amphiphilic random copolymers containing hydrophobic and hydrophilic side chains spontaneously self-assemble in water via hydrophobic interaction into a spherical unimer or multi-chain micelles. We design amphiphilic random copolymers containing a stereocenter in the hydrophobic chain to investigate how molecular chirality can affect the micellar packing in aqueous solution. We synthesize two mirror-imaged hydrophobic monomers and incorporate into the amphiphilic random copolymer via reversible addition-fragmentation chain transfer (RAFT) process. Their chiral effects on self-assembly will be discussed based on the dynamic light scattering (DLS), circular dichroism spectroscopy (CD), and small angle X-ray scattering (SAXS) analyses.

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

Polymer Chemistry

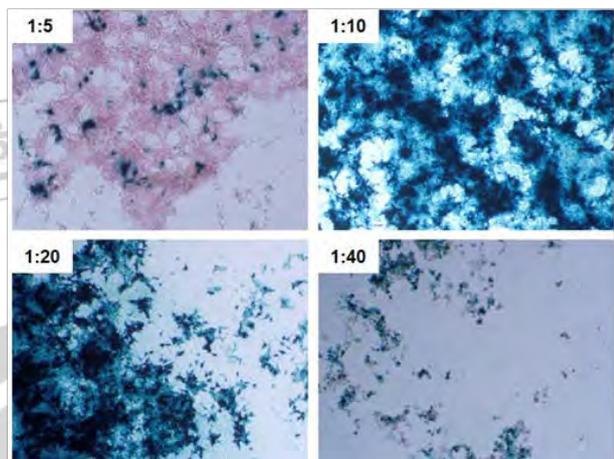
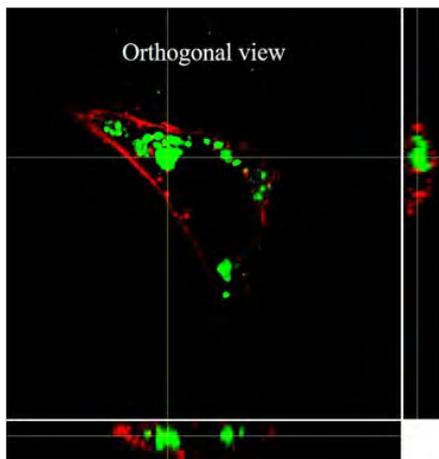
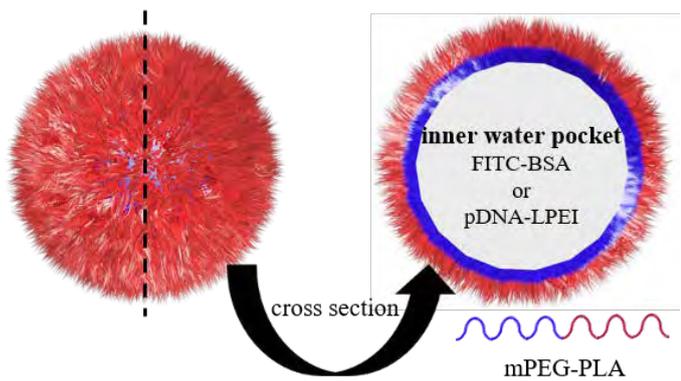
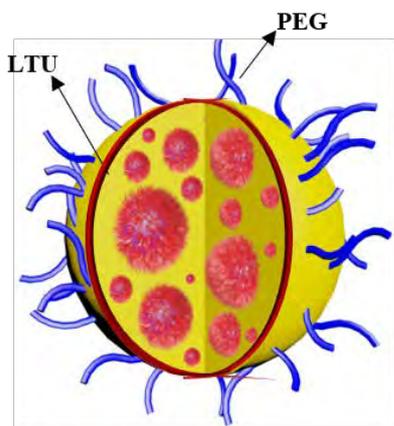
Exhibition Hall 2, FRI 11:00~12:30

Double-Emulsion Nanoparticle Based on L-tyrosine Polyurethane with high bioavailability for Efficient Gene Delivery

Soo Yong Park, Ildoo Chung*

Department of Polymer Science and Chemical 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-7**

Polymer Chemistry

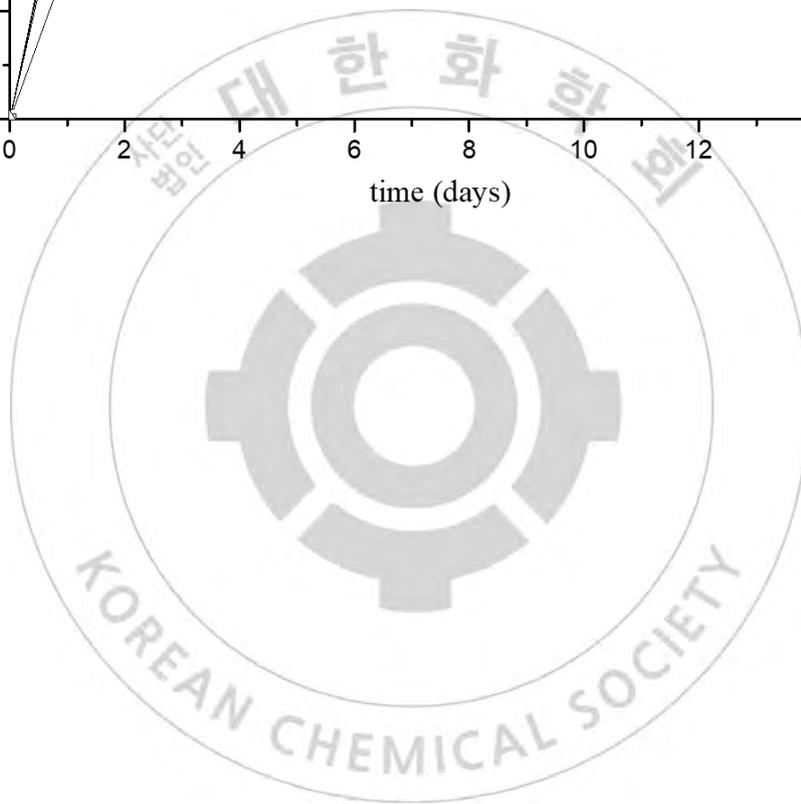
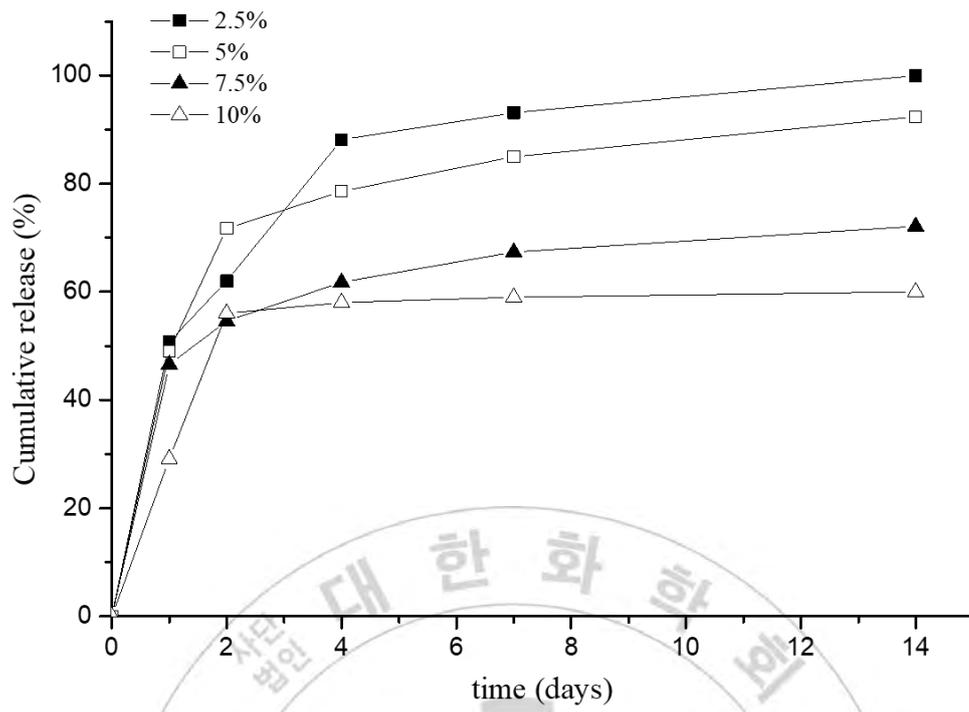
Exhibition Hall 2, FRI 11:00~12:30

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

Soo Yong Park, Ildoo Chung*

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

Biodegradable polyfumarateurethane (PFU) for delivery vehicle using di-(2-hydroxypropyl fumarate) (DHPF), 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-8**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Visualization of Human Hairs; FT-IR and Confocal Microscopic Studies.

Daeyeon Cho, Soo Ryeon Ryu¹, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

¹Department of Chemistry, Biological Interface Labo, Korea

Hair is a protein filament that grows from follicles found in the dermis. Hair is one of the defining characteristics of mammals. We know well about structural information about human hair, but very few parts of physical properties of human hair, such as diffusivity, acidic resistance, etc., are known. Therefore, our ultimate-goal is to unveil secrets of human hair using analytical instruments, especially by FT-IR microspectrophotometer and confocal laser scanning microscopy. FT-IR microscopy can combine visual microscopic hair fiber analysis with valuable and discriminating infrared chemical information. It is also a useful method for the analysis of human hair because it can be used to analyze both the cortex and the cuticle of cross-sectioned hair. Transformations due to the breakage of bonds in specific chemical groups were observed and spatially characterized. Hair fiber chemical information can reveal residual hair styling products, such as hairspray and conditioner, and protein structure changes due to chemical treatments, like bleaching. Confocal microscopy is an excellent method for studying the localization of fluorescent stains. Used in this way, superior 3D images can be obtained from multiple optical sections with very shallow depth of field. Confocal microscopy requires only minimal sampling preparation, and the hair can be observed in its natural environment with less damage than by other microscopic methods such as SEM. This relatively noninvasive, nondestructive technique is routinely used by us to monitor the efficiency of cleansing shampoos, to assess the homogeneity of layering polymers, and to evaluate the changes they induce in the optical properties of the hair surface in terms of opacity, transparency, and brilliancy.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mechanical properties of bio-printed vascular system

Yeongheon Jung, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Despite the significant advancements in bio printing and tissue engineering to mimic native tissue constructs, fabrication of bifurcating vessels and vascularized tissue constructs still pose a great challenge. Previous studies reported various fabricating method of artificial blood vessel which has limitations that control of vessel wall thickness, structural stability, free-standing printed model vasculatures with controlled lumen diameter and wall thickness. The novel method to bioprint bifurcating vessels and develop hierarchical vasculature can overcome the downsides of previous studies. 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. The rheological properties of PFCa ink is defined. The wall thickness of artificial blood vessel depends on the pressure, nozzle size, incubation time are optimized. Artificial blood vessel, physically modified by acrylate and diacrylate, enables various possibilities of implantation and organ-on-a-chip.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Increasing Performance of Organic Field Effect Transistor by adjusting shearing force within eutectic system

SangWon Eom, Jiyun Jung, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

Donor-acceptor type polymers in which electron rich(donor), electron deficient(acceptor) are repeatedly connected to a polymer backbone, have attracted attention in many research fields due to their high electrical characteristic, however donor-acceptor type polymers have difficulties in application because of low solubility in organic solvents and low crystallinity, so based on eutectic system, we have enhanced electron mobility by increasing crystallinity through making nanowire with vertically confined mold and applying shear force to film, further have optimized epitaxial growth condition by controlling the phase separation rate within the microchannel, consequentially this system, which can be easily processed at low temperatures(around 60 °C) and increase the crystallinity, opens up the possibility of device application for donor-acceptor type polymers.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Thermosensitive hydrogel as a 3D cell culture niche

Hanbyul Jang, Heeju Kim, Min Hee Park, Byeongmoon Jeong*

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

Thermogel is an aqueous polymer solution that undergoes sol-to-gel transition as the temperature increases. Cells, growth factors, and signaling molecules can be incorporated simultaneously during the sol-to-gel transition. The cytocompatible procedure makes the thermogel an excellent platform for 3D culture of stem cells. This review focuses on the crucial questions that need to be addressed to achieve effective differentiation of stem cells into target cells, comprising low modulus, cell adhesion, and controlled supply of the growth factors. Recent progress in the use of thermogel as a 3D culture system of stem cells is summarized, and our perspectives on designing a new thermogel for 3D culture and its eventual application to injectable tissue engineering of stem cells are presented.



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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

pH dependence and EDTA treatment impact on catechol modified chitosan hydrogels

Quang Nguyen Ngoc, Daewon Sohn^{1,*}

Chemistry, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Chitosan (CS) is a natural polycationic polysaccharide and pH sensitive polymer with incomplete deacetylation from chitin. It is also a guaranteeing material in terms of pharmaceutical, chemical, and sustenance industry due to its exceptional structure including reactive –OH and –NH₂ groups. In this study, a catechol-functionalized chitosan (CCS) for an eminent level for substitution was synthesized and propelled by marine mussel cuticles in place on research those intricate connections between Fe³⁺ and catechol under acidic conditions. The ratios of catechol, chitosan and other reagents decide the structure of the hydrogel. The gel formation is then well-maintained by dual cross-linking through electrostatic interactions between CCS and oxidative ions such as Fe³⁺ and IO₄⁻ through covalent catechol-coupling-based coordinate bonds. The hydrogels showed enhanced cohesiveness and shock-absorbing properties at lower pH and EDTA treatment due to coordinate bonds inspired by mussel byssal threads. Thus, the gelation time, rheological properties, UV-vis and ¹H- Nuclear Magnetic Resonance spectroscopy, and the morphologic aspects were elucidated to describe those crosslinking components and the physical properties of the chitosan backbones and hydrogel frameworks.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characteristics of PNiPAM hydrogels synthesized by γ -ray irradiation

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¹*Department of Chemistry, Hanyang University, Korea*

The chemical and mechanical properties of poly(N-isopropylacrylamide) (PNiPAM) hydrogels were investigated. Four different methods were used preparing PNiPAM hydrogels; γ -ray was irradiated to monomer-clay solution in direct method (DM), to clay solution in indirect method (IM) and to monomer solution in monomer method (MM), and general method (GM) is synthesized by potassium persulfate (KPS) initiator. γ -ray generates radicals and forms 3-D network without any crosslinker while general method uses N,N'-methylenebisacrylamide as a crosslinker. Swelling properties depending on time was 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 four methods, chemical method showed self-healing property and the best swelling property because of the structural difference. The morphology of PNiPAM hydrogels was also investigated to see microscopic structural using scanning electron microscope (SEM).

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Difference between anisotropic and isotropic particles in flow cytometry

Hoyeon Lee, Daewon Sohn^{1,*}

Graduate student in chemistry, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

As a matter of shapes, most of bacteria have the rod-like shape, whereas red blood cells (RBCs) have the disk-like structure. This research was focused on increasing sensitivity for bacteria exclusively. We could discover the shape difference of bacteria and RBCs by using light scattering technique in flow cytometry. Two different silica particles were used representing bacteria and RBCs. Dependence on the shape of particles for signal intensity has been investigated. Isotropic sphere silica particles representing human red blood cells with three different sizes and anisotropic rod-like silica particles representing bacteria were synthesized. These materials were analyzed with a dynamic light scattering (DLS) and scanning electron microscope (SEM). Samples containing sphere or rod-like particles themselves or their mixtures were measured by using a flow cytometer for the height data of forward scatter (FSC-H), which means intensity of signals. Although radius of gyration of rod-like particles is bigger than sphere particles, it has weaker intensity. The anisotropy of rod-like particles makes this kind of difference. Since sphere particles are isotropic, these particles have the round-shaped scattering pattern. And this isotropic property can keep most scattered signals within the detecting area which can collect signals in practice. In contrast, anisotropic particles form two symmetric lobes when scattering. And the edge of this lobe escape detecting area. In addition, flow cytometry experiments with different ratios of these two particles were also carried out for sensitivity of detection on anisotropic rod-like silica particles. rod-like particles are observed even when it was only about a tenth of round-shaped particles.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Noncovalently Conformational Locking in Indacenodithiophene-based A-D-A type Molecule and Its Application to High-performing Non-fullerene Polymer Solar Cells

Su Hong Park, Hyung Jong Kim, Cheol Hun Jeong, Nayeon Kwon, Ji Hye Lee, Min Ju Cho*, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

A new A-*b*-D-*b*-A-type n-type small molecule, IDT-3MT, was synthesized bearing a weak acceptor thiophene-3-carboxylate bridge (3MT = *b*) between indacenodithiophene as a donating core and 2-(3-oxo-2,3-dihydroinden-1-ylidene)-malononitrile as the accepting end groups. Compared to IDT-T bearing a neat thiophene bridge, IDT-3MT displayed a red-shifted absorption spectrum in the film state, which is a more effective complementary absorption behavior with PBDB-T as the donor material. Methyl-3-thiophenecarboxylate (3MT) moiety with weak electron affinity can lower the LUMO energy level to increase the difference of the LUMO energy levels between the donor and acceptor (ΔE_{LUMO}), and provide enhanced driving force for efficient exciton dissociation resulted as higher J_{SC} in OSCs. Based on the results of grazing-incidence wide-angle X-ray scattering, the blend film of PBDB-T:IDT-3MT exhibited a more prominent face-on orientation and fine surface morphology compared with PBDB-T:IDT-T, which can facilitate charge transportation in the vertical direction. Among two acceptors, as-cast blend film (solvent additive free) of PBDB-T and IDT-3MT exhibited the highest power conversion efficiency of 8.40 % due to complementary absorption and favorable internal morphology in application of polymer solar cell.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Random Conjugated Terpolymers for High-Efficient Non-Fullerene Polymer Solar Cells

Min Ju Cho, Su Hong Park, Nayeon Kwon¹, Youngun Kim, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

¹*Chemistry, Korea University, Korea*

Bulk heterojunction polymer solar cells (PSCs) have been considered ideal for application in large-area flexible devices fabricated via low-cost practical solution processes such as spin-coating, ink-jet, and roll-to-roll printing techniques. Among many kinds of conjugated polymers, random terpolymers have emerged as promising materials with many advantages over electron-donating binary copolymers owing to the ability to fine-tune the internal morphology of the active layer, solubility, absorption range, energy levels, and polymer chain orientation of the former in blend films. In this work, a new conjugated terpolymers based on 4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene as the electron-donating unit, methyl-3-thiophenecarboxylate (3MT) as the weak electron-accepting unit, and benzo[c][1,2,5]thiadiazole (BTz) or 5,50-bis(2-ethylhexyl)-4H,4'H-1,10-bithieno[3,4-c]pyrrole-4,4',6,6'(5H,5'H)-tetraone (BiTPD) as the electron-accepting unit stronger than 3MT were synthesized to investigate the effect of the BTz or BiTPD unit on their optical and electrochemical properties and the performance of the derived non-fullerene PSC devices.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Diketopyrrolopyrrole-Based Conjugated Polymers bearing Branched Alkyl Ester-Labeled Side Chains and their Thin Film Transistors

Hyung Jong Kim, Su Hong Park, Cheol Hun Jeong, Nayeon Kwon, Ji Hye Lee, Min Ju Cho*, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

Recently, many studies have focused on improving the carrier mobility in organic thin film transistors (OTFTs) by optimizing the size and bifurcation points of bulky branched alkyl chains on the conjugated backbone segments. However, it is difficult to prepare these alkyl groups because of their complicated synthesis routes. Additionally, there are limited studies related to the structures of DPP-based copolymers including alkyl side chains with polar functional units, which can induce other interactions besides van der Waals interactions. In this study, we synthesized six different DPP-based copolymers including DPP and bithiophene (BT) as electron-acceptor and donor backbone units, respectively, containing branched alkyl side chains, which were either directly coupled to the N-positions of DPP or separated by an alkyl ester group. It was found that the ester moieties form pseudo-hydrogen bonds with the nearest side chains in comparison to the alkyl-only system. The optimal DPP-based copolymer film showed the highest μ value of $2.30 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ in an OTFT, with a high on/off current ratio ($I_{\text{on}}/I_{\text{off}} > 10^6$).

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

High-performing fullerene free polymer solar cell fabricated by a simple process using new conjugated terpolymers

Jihyun Kim, Youngun Kim, Jiwon Yoon, Chae Yeong Kim, Min Ju Cho, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

Recently, terpolymers showed the several desirable attributes-such as high solubility, broad absorption range, finely tuned energy levels, and improved nanophase internal morphology and orientation of polymer chains in the blends over binary copolymers bearing one each of the donor and acceptor monomeric units. In this study, A series of conjugated terpolymers, P2-P4, based on 4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene as the electron-donating unit, methyl-3-thiophenecarboxylate (3MT) as the weak electron-accepting unit, and 1,3-bis(2-ethylhexyl)benzo[1,2-c:4,5-c']dithiophene-4,8-dione (BDD) as the strong electron-accepting unit were synthesized to investigate the effect of the contents of 3MT and BDD on their optical and electrochemical properties and the performance of the derived fullerene-free polymer solar cell (PSC) devices. Among the three terpolymers, the as-cast blend film of P3:acceptor with complementary absorption and favorable internal morphology exhibited the highest power conversion efficiency of 10.26% with a high open circuit voltage of 0.94 V and short circuit current density of 17.18 mA cm⁻² in the PSC.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Study on photophysical properties of new conjugated polymers bearing macromolecular donor and acceptor monomers.

Nayeon Kwon, Su Hong Park, Hyung Jong Kim, CheolHun Jeong, Ji Hye Lee, Min Ju Cho, Sunnam Park*, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

A wide variety of donor-acceptor(D-A) type small molecule dyad systems have been synthesized and studied to investigate the photophysical properties for a long time. However, the most studies used by the small molecules, the small molecule donor and fullerene acceptors system, and only a few studies exist that relate the physical properties of D-A type polymers. In this study, we have designed and synthesized the uniform macromolecular donor and acceptor monomeric units, and utilized them to synthesize two different type polymers such as, (D- σ -A) $_n$ and (D- π -A) $_n$. (D- σ -A) $_n$ is a partially conjugated polymer, in which the donor is connected to the acceptor through a non-conjugated flexible alkyl spacer. Whereas, (D- π -A) $_n$ is a fully conjugated polymer, in which the donor is connected to the acceptor via π -conjugated spacer. Both polymer's photophysical properties such as, fluorescence quenching, energy transfer and charge transfer were characterized via time resolved spectroscopy.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solution Processed Multi-Layered Organic Light-Emitting Diodes by Using New Crosslinkable Hole Transport Polymer

Ji Hye Lee, CheolHun Jeong, Hyung Jong Kim, Su Hong Park, Nayeon Kwon, Min Ju Cho, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

Besides vacuum processed organic light-emitting diodes (OLEDs), solution processed OLEDs have many advantages such as low-cost, large area, and flexible display application. Despite these advantages, it is difficult to fabricate multi-layered device structure by using the solution-process. The problem is hard to prepare all the layers via solution processing because the bottom layer can be dissolved by the upper layer solvent. The best solution is to use crosslinkable materials for the desired layers. It can be prevented from dissolving in common solvents. In this work, a new crosslinkable hole transport polymer, X-2Cz was synthesized by using the addition polymerization. Solvent resistance of X-2Cz was investigated by using the UV-vis absorption spectroscopy. The results demonstrate that X-2Cz is suitable for use as an hole transport layer in solution process OLEDs.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Single Component Active Layer Polymer Solar Cells with New Conjugated Copolymer Bearing Donor and Acceptor Blocks

Su Hong Park, Hyung Jong Kim, Cheol Hun Jeong, Nayeon Kwon, Ji Hye Lee, Min Ju Cho, Sungnam Park*, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

A new conjugated copolymer bearing donor and acceptor blocks (O-BCP) for the single component active layer was successfully synthesized based on a relatively facile synthesis process which is high yield through one-pot polymerization and purification. The O-BCP contains PBDT-EH2T of p-type units and PNDI-Se of n-type blocks along the polymer chains. All properties of O-BCP were compared with those of blend samples of PBDT-EH2T and PNDI-Se. A single component active layer-PSCs based on as-cast film exhibited a PCE of 2.62%. ($V_{oc} = 0.77$ V, $J_{sc} = 8.90$ mA/cm², FF = 43.93%). However, through the thermal treatment at 180 °C for 10 min, the devices performance was remarkably improved to show intriguingly high J_{sc} and FF resulting in >4.57% of PCE. Compared to the O-BCP, the blend film displayed a relatively poor efficiency. ($V_{oc} = 0.72$ V, $J_{sc} = 6.28$ mA/cm², FF = 43.04%, PCE = 1.94%).

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

Polymer Chemistry

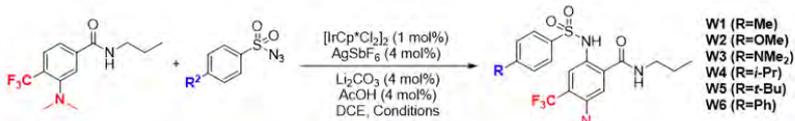
Exhibition Hall 2, FRI 11:00~12:30

White-Light-Emitting Polymer via Iridium-Catalyzed Direct C-H Amidation Polymerization: A Strategy Utilizing Excited-State Intramolecular Proton Transfer

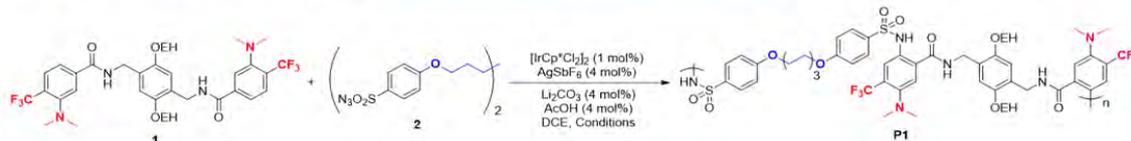
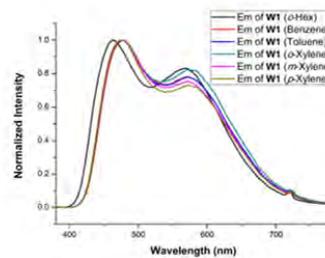
Soon-Hyeok Hwang, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

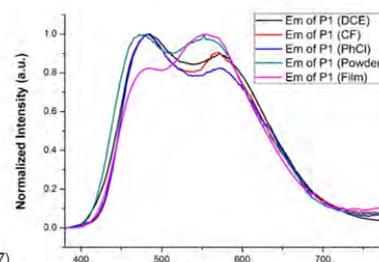
Recently, we reported iridium-catalyzed direct C-H amidation polymerization (DCAP) to produce polysulfonamides emitting blue-light via excited-state intramolecular proton-transfer (ESIPT). Since the start of ESIPT research, some strategies have been reported to create white-light (WL)-emitting small molecules. However, WL-emitting polymer via ESIPT has not been reported so far. Herein, we reports the first example of WL-emitting polymer in both solution- and solid-states via ESIPT, resulting from DCAP. From the viewpoint that fluorophores are produced during the polymerization process, DCAP has a distinctive difference from other polymerizations using monomers that already contain fluorophores. To get WL emission which can be obtained by thermal equilibrium between blue-emitting N* and yellow-emitting T* with proper intensity ratio, small molecule studies were conducted by screening solvents as well as changing the electronics and positions of substituents on aryl rings. After getting successful WL in small molecules, W1-W6, based on the structures of coupling partners for W1-W6, AA-type and BB-type monomers were designed to make WL-emitting polymers. Resulting P1 via DCAP could give WL emissions successfully in some solvents, which can induce thermal equilibrium between N* and T* with proper intensity ratio as well as in solid state. DCAP using proper monomers could give WL-emitting polymer via ESIPT regardless of phases, i.e., solution and solid. In other words, even in ESIPT field, WL-emitting film, which has been made using WL-emitting small molecule and polymer matrix, can be obtained without other polymer matrix. Thus, this DCAP provides an opportunity to use WL-emitting polymer via ESIPT for applications such as displays and light source.



Solvent	CIE Coordinates	Solvent	CIE Coordinate
c-Hex	(0.31, 0.34)	o-Xylene	(0.32, 0.36)
Benzene	(0.32, 0.37)	m-Xylene	(0.31, 0.36)
Toluene	(0.32, 0.36)	p-Xylene	(0.31, 0.35)



Solvent	$\lambda_{\text{max, em}}$ (nm)	Relative QY	CIE Coordinates
DCE	N : 484, T : 572	0.12	(0.33, 0.38)
CF	N : 482, T : 568	0.12	(0.33, 0.39)
PhCl	N : 482, T : 572	0.12	(0.33, 0.38)
Powder	N : 472, T : 552	0.16 ^a	(0.31, 0.37)
Film	N : 486, T : 556	-	(0.33, 0.41)



^a Absolute QY (Average value of three values; 0.1600, 0.1561, and 0.1567)



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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Thermally Crosslinkable Hole Transport Polymer for Realizing High-Performing Thermally Activated Delayed Fluorescence OLEDs via Solution Processing

Cheol Hun Jeong, Jiwon Yoon, Hyung Jong Kim, Su Hong Park, Chae Yeong Kim, Nayeon Kwon, Ji Hye Lee, Min Ju Cho, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

Recently, solution processable organic light-emitting diodes (OLED) have emerged as alternative to vacuum processed OLEDs due to the low-cost, large area, and flexible display applications. However, it is still difficult to prepare all the layers in multi-layered OLEDs via solution processing since bottom layer can be dissolved during the deposition of the upper layer. As a solution, crosslinking system has been considered as one of the most effective methods to make insoluble from many common organic solvents without any complicated fabrications. A new side-chain hole transport polymer, X-TPACz which contains thermally crosslinkable side chain unit, was synthesized via facile addition polymerization. Using the UV-vis absorption spectroscopy, curing conditions were optimized by investigation in terms of curing temperature and curing time. Using X-TPACz as hole transport layer, high external quantum efficiency with low turn on voltage was obtained in application of solution processable OLED.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Polaron Dynamics of a Non-Fullerene Acceptor in Ternary Blend Organic Solar Cells

Dongki Lee, Kilwon Cho*

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

We investigated the extension effects of side-group and backbone of a push-pull conjugated polymer (CP) on ternary-blend organic solar cells (OSCs) containing PC₇₁BM and a non-fullerene acceptor (NFA). The photovoltaic properties of the OSCs prepared with the side-group (PBTBT-OTT) and backbone (PDTBT-OTT) extended CPs are strongly dependent on the additional free carriers (FCs) that are generated from the NFA. Especially, PDTBT-OTT induced the ultrafast charge-transfer to PC₇₁BM due to the efficient intrachain energy-transfer, which resulted in the unique formation-pathway of the additional FCs in the NFA domains. This phenomenon enhanced photocurrent of the ternary-blend NFA OSC with PDTBT-OTT by complementing the nongeminate recombination losses between PDTBT-OTT and the acceptors.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Properties of Piperidinium and Pyrrolidinium PEG copolyesters

Hyun Ho Chae, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

A series of polyesters containing piperidinium or pyrrolidinium cations with PF₆ or Tf₂N counter-anions and poly(ethylene glycol) (PEG-400, 1000 or 4000) units on a backbone are successfully synthesized from dihydroxyl piperidinium/pyrrolidinium room temperature ionic liquid monomers. After using equimolar ratio of dihydroxyl ionic liquid monomers and PEG for polyesterifications, 1:1:2 ratio of the cation units, PEG segments and sebacate units in the copolyesters is confirmed by ¹H NMR. Differential scanning calorimetry measurements reveals that ionic polyesters with higher molecular weight PEG and with longer alkylene moieties result in crystallization during either a heating or cooling scan. Thermal stabilities of the synthesized copolyesters are confirmed by TGA and the synthesized ionic copolyesters are mostly stable up to 300 °C.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Properties of Pyrrolidinium Polyurethanes from Ionic-Liquid Monomers

JongChan Shin, Minjae Lee^{1,*}

Kunsan National University, Korea

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

Novel polyurethane ionomers are synthesized using hydroxyl pyrrolidinium ionic liquid monomers. Ionic polyurethanes with different diisocyanates, such as [Methylenedipheny 4,4'-diisocyanate](MDI), [Tolylene-2,4-diisocyanate](TDI) and [Dicyclohexylmethane 4,4-disocyanate](HMDI) are investigated about their chemical and physical properties by different spacers. Also, different anions, such as Br⁻, Tf₂N⁻, and PF₆⁻ are used for the ionic polyurethanes and they are characterized to see the different properties. The pyrrolidinium bromide-based polyurethanes with TDI spacers has the lowest glass transition temperature (T_g), 37 °C on its different scanning calorimetry thermogram. From thermal gravimetry experiments, the Tf₂N⁻ polyurethanes show a higher thermal stability and lower T_g.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Hyper-Cross-Linked Polymer with Enhanced Porosity by in situ Removal of Functional Groups

Jeonghyeon Lee, Myungeun Seo^{1,*}

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

¹*Graduate School of NanoScience and Technology, Korea Advanced Institute of Science and Technology,
Korea*

Hyper-cross-linked polymers (HCPs) contains micropores (pore size < 2 nm) within a densely cross-linked aromatic framework. For example, Lewis acid-catalyzed electrophilic aromatic substitution (i.e., hyper-cross-linking reaction) between the aromatic rings in poly(4-vinylbenzylchloride-co-divinylbenzene) (P(VBzCl-co-DVB)) arrests free volume into permanent microporosity with high specific surface area. To control the pore characteristic of HCPs, we recently reported a unique methodology based on incorporation of a trimethylsilyl (TMS) group into P(VBzCl-co-DVB). The in situ removal of the bulky TMS groups during the hyper-cross-linking reaction results in the enhanced porosity. Herein, we explore various functional groups as molecular templates to micropore creation in the HCP. By synthesizing functional group-containing styrenic monomers and hyper-cross-linking the functional-group containing precursors, we will present influence of the functional groups on the pore characteristics.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Co-oligomerizations of 2,5-Dibromo-1,1-diisopropyl (or dihexyl)-3,4-diphenyl-siloles with 4,4'-(Hexafluoroisopropylidene)diphenol or 4,4'-Biphenol and their Characterizations

Jong Wook Lim, Young Tae Park^{1,*}

Keimyung University, Korea

¹*Department of Chemistry, Keimyung University, Korea*

2,5-Dibromo-1,1-diisopropyl (or dihexyl)-3,4-diphenyl-siloles as monomers were prepared by intramolecular reductive cyclization reactions of diisopropyl (or dihexyl)-bis(phenylethynyl)silanes using lithium naphthalenide, anhydrous ZnCl₂, and *N*-bromosuccinimide (NBS), respectively. Co-oligomerization reactions of 2,5-dibromo-1,1-diisopropyl (or dihexyl)-3,4-diphenyl-siloles with 4,4'-(hexafluoro-isopropylidene)diphenol or 4,4'-biphenol were carried out by the nucleophilic substitution reaction of two bromine groups in the presence of potassium carbonate under the solvent of *N*-methyl-2-pyrrolidinone (NMP) and toluene by azeotrope using Dean-Stark trap. The crude oligomeric products were purified by extraction using the solvents of tetrahydrofuran and dichloromethane, and washed with deionized water. The oligomeric product materials were characterized by ¹H, ¹³C, and ²⁹Si NMR as well as GPC. We also studied the photoelectronic properties by UV-vis absorption, excitation, and fluorescence emission spectroscopic methods, 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 : **POLY.P-29**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Transformation of Poly(4-vinylphenol)-b-Poly(vinyl alcohol) diblock copolymeric micelle in Mixed Solvent Systems

Taehyoung Kim, Sang Youl Kim*

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

Due to the different affinity of poly(4-vinylphenol) and poly(vinyl alcohol) with solvents, the diblock copolymer consisting of these two polymers can be self-assembled into a core-shell type particle. We synthesized poly(4-vinylphenol)-b-poly(vinyl alcohol) diblock copolymer and studied the core-shell structure in mixed solvent systems. The poly(4-vinylphenol) and the poly(vinyl alcohol) blocks were obtained by hydrolyzing their precursor, poly(4-acetoxystyrene) and poly(vinyl acetate), respectively. In water/DMSO mixed solvent condition, we confirmed the core-shell structure in which poly(4-vinylphenol) block acts as a core and poly(vinyl alcohol) block acts as a shell. In contrast, the core-shell particle with the inverted composition, poly(vinyl alcohol) core and poly(4-vinylphenol) shell, was formed in the THF/DMSO mixed solvent system. Interestingly under the condition of THF/DMSO mixed solvent system, we could observe other morphologies of core-shell nanoparticles besides spherical micelle. From the change of fluorescent emission shape and metal-polymer interaction in different solvents, the location of poly(4-vinylphenol) block can be identified.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Biocompatible Nitrogen Containing Aliphatic Polymer: Electron Transfer based Singlet Oxygen Generator for Photodynamic Therapy

Jung seung Nam, Chaiheon Lee¹, Byeong-Su Kim^{2,*}, Tae-Hyuk Kwon^{3,*}

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

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

²*Department of Chemistry, Yonsei University, Korea*

³*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

Singlet oxygen generators containing conjugated aromatic group or heavy metal atom have shown good efficacy in PDT, however, the most of materials have had limitations as therapeutic agents because of their poor biocompatibility. Herein, we introduce new type of singlet oxygen generator based on nitrogen of aliphatic polyamino glycerols (PAG), which have excellent biocompatibility. It was confirmed that nitrogen atom on backbone was the source of electron transfer owing to its paramagnetic properties and that generates radical oxygen species ($O_2^{\cdot-}$, HO_2^{\cdot} , or H_2O_2), subsequently converted to singlet oxygen. Additionally, PAG successfully ablated cancer cells by photodynamical pathway.

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

Polymer Chemistry

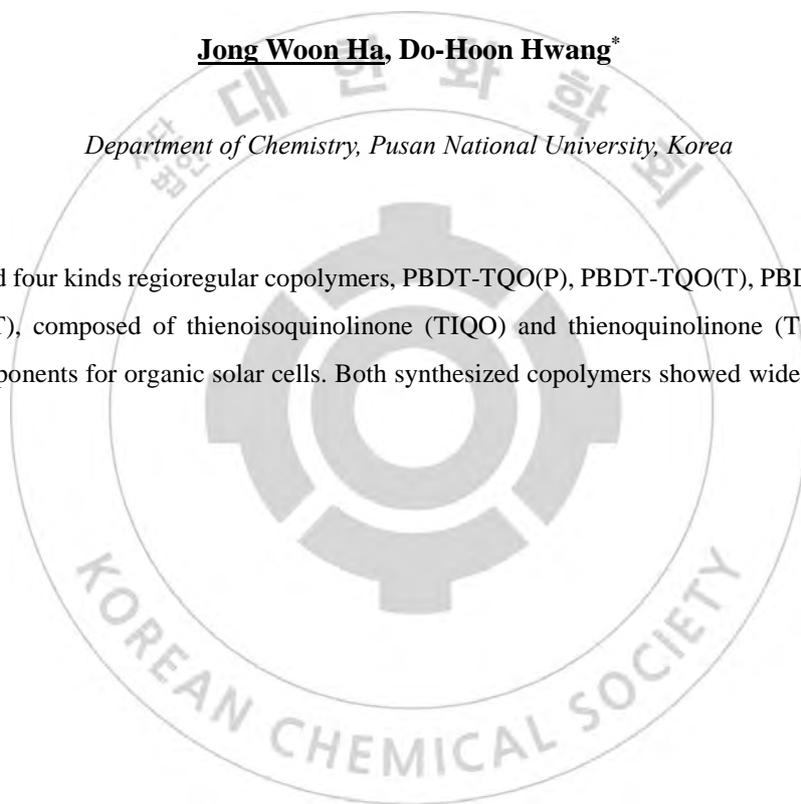
Exhibition Hall 2, FRI 11:00~12:30

Regioregular Wide Bandgap Copolymers Based on Thienoisquinolinone and Thienoquinolinone for Efficient Non-Fullerene Organic Solar Cells

Jong Woon Ha, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

We synthesized four kinds regioregular copolymers, PBDT-TQO(P), PBDT-TQO(T), PBDT-TIQO(P) and PBDT-TIQO(T), composed of thienoisquinolinone (TIQO) and thienoquinolinone (TQO) as electron accepting components for organic solar cells. Both synthesized copolymers showed wide optical bandgap (



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

Polymer Chemistry

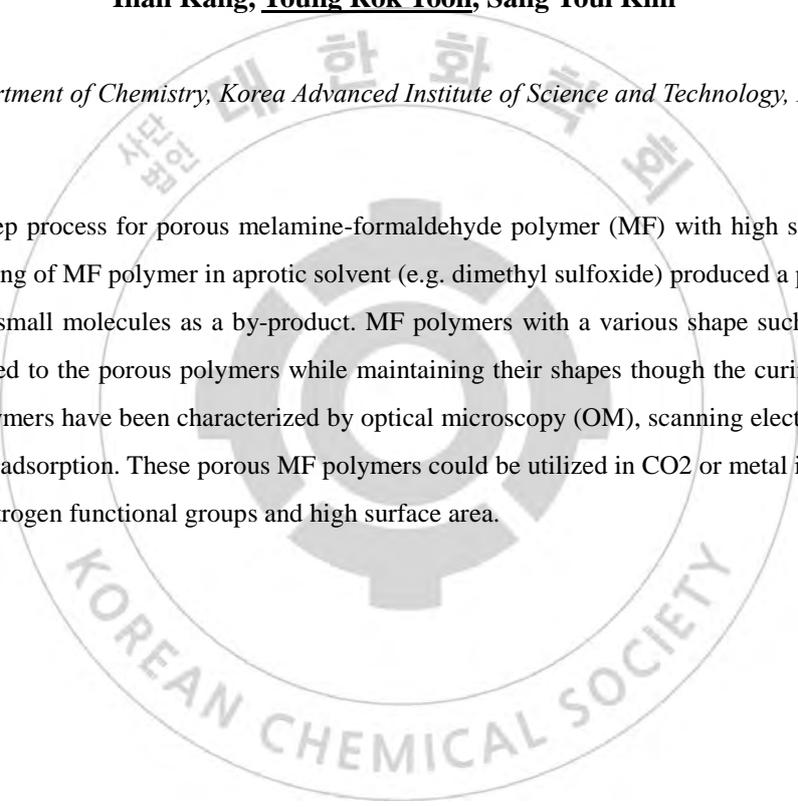
Exhibition Hall 2, FRI 11:00~12:30

Preparation of Shape-controlled Porous Melamine-formaldehyde Polymers

Inah Kang, Young Rok Yoon, Sang Youl Kim*

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

A novel two-step process for porous melamine-formaldehyde polymer (MF) with high surface area was developed. Curing of MF polymer in aprotic solvent (e.g. dimethyl sulfoxide) produced a porous structure by eliminating small molecules as a by-product. MF polymers with a various shape such as particles or rods, transformed to the porous polymers while maintaining their shapes though the curing process. The porous MF polymers have been characterized by optical microscopy (OM), scanning electron microscopy (SEM), and N₂ adsorption. These porous MF polymers could be utilized in CO₂ or metal ion capture with the abundant nitrogen functional groups and high surface area.



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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Compartmentalized Bimetal Nanostructures for Photonics-based Biosensing

Eun Young Hwang, Dong Woo Lim^{1,*}

Bionano Technology, Hanyang University, Korea

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

Compartmentalized bimetal nanostructures have distinct surface properties as well as unique plasmonic properties at each metallic compartment, as compared to those of the single metallic counterparts. Especially, surface-enhanced Raman scattering (SERS) has been of great importance for biochemical detection because it has ultra-high sensitivity, narrow bandwidth as well as significant multiplexing capabilities. Herein, we report synthesis of core-shell, eccentric- and heterodimeric bimetal nanostructures with anisotropy via competitive ligand coordination between two immiscible ligands at different molar ratios. Both hydrophobic- and hydrophilic ligands were competitively bound to Au seeds asymmetrically, and Ag ions were simultaneously reduced, forming into the second Ag metallic compartment onto the Au seeds. A diblock copolymer as a ligand was synthesized via reversible addition-fragmentation chain transfer polymerization, and catechol groups were chemically conjugated with its hydrophilic block. In addition, to prove that these bimetal nanostructures could serve as SERS nanoprobe for biosensing applications, we demonstrated the formation of sandwich-type immunocomplexes composed of SERS nanoprobe and magnetic beads in the presence of target proteins, and showed SERS-based quantitative analysis. Conclusively, this work has great potential as multi-functional nanostructures for SERS-based biosensing.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Organic-Inorganic Nanocomposites based on Self-assembled, Fusion Protein Nanostructures for Theragnosis

Min Jeong Kang, Aamna Basheer, Dong Woo Lim^{1,*}

Department of Bionanotechnology, Hanyang University, Korea

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

Organic-inorganic nanocomposites based on protein nanostructures have been of growing interest for nanomedicine applications. In this study, we report self-assembled, fusion protein nanostructures and growth of metallic nanoparticles (MNPs) within them for theragnosis. The fusion proteins composed of penta-helices for self-assembly, thermally sensitive elastin-based polypeptide (EBP) and two different antiangiogenic peptides (AFs) for inhibition of angiogenesis were genetically engineered, expressed and purified by using non-chromatographic purification method. Furthermore, MNPs were grown within the protein nanostructures via metal ion binding and subsequent reduction for diagnosis of angiogenesis. Thermal-sensitivity and self-assembly of fusion proteins as well as MNP synthesis were characterized by UV-Vis absorbance, dynamic light scattering and transmission electron microscopy. This work suggests that fusion protein-based composite nanostructures would have great potential for theragnosis in angiogenesis-related diseases.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Acorn-Shaped Bimetal Nanoparticle Clusters for Surface Enhanced Raman Scattering-based Biosensing

Jae Hee Lee, Eun Young Hwang, Dong Woo Lim^{1,*}

Department of Bionanotechnology, Hanyang University, Korea

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

Compartmentalized bimetallic nanoparticles have gained great interest to exploit unique optical properties for biosensing applications. Asymmetric distribution of chemical functionalities, composition and effective coupling of different metal domains would be promising as optical nanoprobe due to different physicochemical- and optical properties depending on the shape and size. We report herein synthesis of acorn-shaped bimetal nanoparticles (ASBNs) prepared by polyol method and their clustered structures induced by noncovalent interactions to develop SERS nanotags with controlled architectures. The ASBNs were prepared through overgrowth from functionalized gold seeds with octadecylamines, and their acorn shape was largely controlled by ammonia, surfactant, temperature, and reaction time. Their clustering was achieved by hydrophobic interactions of octadecylamines on the seed surface of the ASBNs. The ASBN clusters showed highly enhanced SERS intensity as compared to that of single ASBNs. Conclusively, these ASBN clusters would be advantageous as functional SERS nanoprobe for biosensing applications.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photo-chemically Cross-linked Hydrogels of Elastin-Resilin Block Copolypeptides for Biomedical Applications

Aamna Basheer, Min Jeong Kang, Jae Hee Lee, Dong Woo Lim^{1,*}

Department of Bionanotechnology, Hanyang University, Pakistan

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

Photo-initiated, chemically-crosslinked polypeptide hydrogels have been of growing interest for biomedical applications because they have significant advantages including biodegradable polypeptides, fast curing rates with biocompatible precursors under physiological conditions, and generation of minimized heat. In this study, we report photo-chemically cross-linked of elastin-resilin triblock copolypeptides composed of thermally responsive elastin-based polypeptide (EBP) as an end block and resilin-based polypeptides (RBP) with resilient property as a hydrophilic middle block. As temperature increased, EBP end block was aggregated into hydrophobic domains and tyrosine residues of RBP middle blocks were then photo-chemically cross-linked in the presence of photo-catalyst via UV irradiation within several minutes. As characterized by rheological experiments, these hydrogels showed enhanced mechanical properties including complex shear modulus, equilibrium shear modulus and equilibrium compressive modulus as compared to those of the physically crosslinked ones. In conclusion, these block copolypeptide hydrogels would be promising for tissue engineering and regenerative medicine applications.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Evaluation of Physical Properties of High Performance Ophthalmic Lens Containing Hyaluronic Acid and Graphene Oxide Nanocolloids

Jae-wuk Seok, Subin Park, A-Young Sung*

Department of Optometry, Daegu Catholic University, Korea

This experiment was performed to compare the physical properties of Hyaluronic acid and Graphene oxide nanocolloids for the hydrogel lens material. AIBN (Azobisisobutyronitrile) was used as an initiator with HEMA (2-Hydroxy ethyl methacrylate) and EGDMA (Ethylene glycol dimethacrylate) as a basic combination. Hyaluronic acid (HA) was fixed at 5% as an additive, and Graphene oxide nanocolloids were added gradually increasing from 0.1% to 0.5%. The hydrogel lenses were prepared by thermal polymerization at 100 °C for 1 hour. The refractive index tended to be lowered from 1.4358 to 1.4149. In case of Graphene oxide nanocolloids, there was no significant difference from that of Ref (HEMA combination). However, as the amount of Graphene added increased, the fluctuation of refractive index decreased rapidly. The water content tended to increase with the addition of 0.1% Graphene, which was 38.91% ~ 40.55%, but it increased rapidly from 40.55% to 44.23% as the amount of Graphene oxide nanocolloids was increased. As a result of physical properties of produced lens, refractive index of contact lens with hyaluronic acid and Graphene oxide nanocolloids showed a tendency to decrease and water content tended to increase. Especially, as the amount of Graphene oxide nanocolloids increased, the fluctuation of physical properties was increased. Therefore, this material is considered to be suitable as a material for hydrogel lenses.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Conformation-controlled Supramolecular Polymerization of Host-guest Complexes

**Seoyeon Choi, Rahul Dev Mukhopadhyay^{1,*}, Wooseup Hwang², Kangkyun Baek^{3,*},
Kimoon Kim^{2,*}**

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¹*Center for Self-assembly and Complexity (CSC), Institute for Basic Science (IBS), Korea*

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Supramolecular polymers are easy to handle due to their low viscosity, resulting from the polymeric arrays of monomer units, held together by reversible non-covalent interactions. However, most supramolecular polymers are formed by a step-growth mechanism wherein it is difficult to attain uniform polymer chain growth and dispersity. Very recently, supramolecular systems, which undergoes a living polymerization process, has gained attention to overcome the aforementioned issues. In the living polymerization process, the last monomer unit on each polymeric array remains active until all monomer units are consumed completely and acts as an initiating point or seed for a new polymeric chain. Cucurbit[8]urils are known to form heteroternary complexes through charge-transfer interactions inside their hydrophobic cavity. The competitive exchange between guests, due to different association constants can be utilized to switch between different host-guest complexes. Herein, we have designed guest molecules consisting of donor and acceptor parts bridged by linkers, which are flexible enough to initiate polymer growth by undergoing a conformational change in presence of minuscule amount of a competing guest molecule. The formation of the heteroternary complex in solution and supramolecular polymer growth were investigated using various spectroscopic and microscopic techniques as well as computational simulations. Whether this unique supramolecular polymerization can be further exploited as a system undergoing living polymerization is currently under progress. This study may expand the scope of application of supramolecular host-guest chemistry and achieve better control over supramolecular polymerization.

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

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

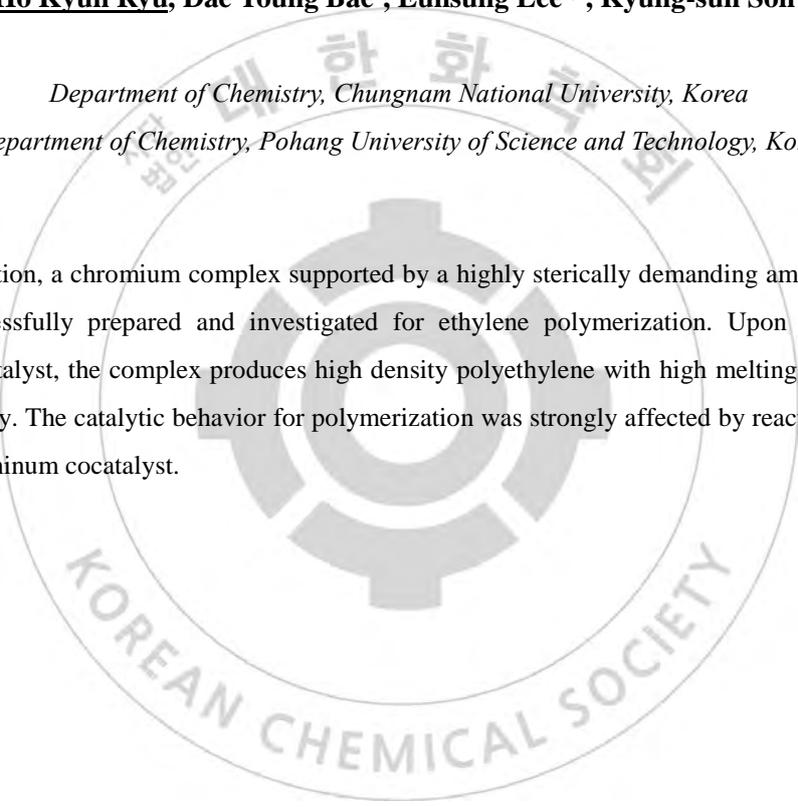
High Density Polyethylene Production by Chromium Complex Based on a Sterically Demanding Ligand

Ho Kyun Ryu, Dae Young Bae¹, Eunsung Lee^{1,*}, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

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

In this presentation, a chromium complex supported by a highly sterically demanding amino triphenolate ligand is successfully prepared and investigated for ethylene polymerization. Upon activation with aluminum cocatalyst, the complex produces high density polyethylene with high melting temperature and high crystallinity. The catalytic behavior for polymerization was strongly affected by reaction solvent and the type of aluminum cocatalyst.



Poster Presentation : **POLY.P-40**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Structure-property-performance Relationships of Organic Photocatalysts for Atom Transfer Radical Polymerization

Chung Soo Kim, Jisu Back¹, Eunsung Lee^{1,*}, Kyung-sun Son^{*}

Department of Chemistry, Chungnam National University, Korea

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

In this presentation, the metal-free atom transfer radical polymerization (ATRP) process mediated by visible light and catalyzed by new organic photocatalysts (PCs) is investigated. The new PCs, designed by diversifying N-aryl phenoxazine, are analyzed and evaluated for organocatalyzed ATRP (O-ATRP) experimentally and theoretically. The structure–property–performance relationships of PCs are investigated to determine the key parameters required for a good PC for use in O-ATRP. The scope of this process is explored in terms of monomer substrates, initiators, and solvents using our new PC. Finally, a well-defined amphiphilic block copolymer is prepared using this method to form micelles, providing a basis for future biomedical applications.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mesoporous Polymer on Metal-Organic Framework

Nam Young Ahn, Jooyeon Lee¹, Myungeun Seo^{*}, Min Kim^{1,*}

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

¹Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs) are crystalline microporous materials constructed by coordination bonding between metal ions or cluster and organic linkers. Their high porosity, high specific surface area, tunable pore size and shape, and functionalizable organic linkers have been appealing for many advanced applications including catalysis and separation. In addition, composite material of MOF and polymers has been extensively studied for introducing new characteristics and applications. In this presentation we will discuss a synthetic route to creation of mesoporous polymer-MOF composites. Synthetic details as well as characterization of new materials will be presented.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Antimicrobial Peptide Mimetic Functional Polyethers

Minseong Kim, Byeong-Su Kim^{1,*}

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

¹*Department of Chemistry, Yonsei University, Korea*

Antimicrobial peptide (AMP) is one of the key components of the immune system found in various organisms. The main mechanism is known to attach and destroy the bacterial cell membrane or to penetrate the cell membrane and inhibit cell metabolism. The cell membrane of the bacteria is known to have a negative charge and hydrophobic bacterial cell phospholipids, thus many AMPs possessed positively charged amino acids and hydrophobic amino acid residues. To date, there have been active investigations to imitate these peptides and build new artificial systems that complement their disadvantages such as proteolysis, low in vivo efficacy, and hemolytic behavior. Poly(ethylene glycol) (PEG) is the best known polyether widely used in various biomedical applications. Similarly, polyether-based polymers synthesized through functional epoxide monomers are anticipated to display similarly high hydrophilicity, flexibility, and biocompatibility. In this study, we design and synthesize a novel AMP mimetic polyethers by using three functional epoxide monomers mimicking natural amino acid. Specifically, azidobutyl glycidyl ether (ABGE) mimicking lysine, isobutyl glycidyl ether (IBGE) mimicking leucine, and 1-ethoxyethyl glycidyl ether (EEGE) mimicking serine. All monomers are successfully synthesized and copolymerized by anionic ring-opening polymerization (AROP). Their biological activities toward diverse bacteria are determined by measuring the minimum inhibitory concentration (MIC). Moreover, the hemolytic concentration (HC50) toward human red blood cell are assayed to ensure the safety of the prepared AMP-mimetic polyethers. We anticipate the potentials of designer epoxide monomers for the synthesis of functional polyethers toward peptidomimetics.

Poster Presentation : **POLY.P-43**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis, and properties of trimers with aromatic heterocyclic compound

Minsub Kim, Intae Kim*

Department of Chemistry, Kwangwoon University, Korea

In this work, we compared two types of trimers synthesized in our laboratory. One is a trimer substituted on both sides with thiophene and the other is a trimer with both substituted selenophenes. We compared the factors related to the conductivity of two trimers. The structure of the compounds was identified by ¹H NMR, ¹³C NMR, and FT-IR spectroscopy. We also posted each UV-vis absorption, cyclic voltammetry(CV), photoluminescence(PL) spectra for the synthesized compounds. Through this work, we can check the efficiency of each trimers 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-44**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of low MW styrene maleic anhydride copolymers as asphaltene dispersants

Joon-Seop Kim*, **Ki - Cheol Song**¹

Department of Polymer Science and Engineering, Chosun University, Korea

¹*Department of Renewable Energy Convergence, Chosun University, Korea*

In this study, the effect of partially amidized styrene maleic anhydride (SMA) copolymer (MW = 7500, S/MA = 2/1) on asphaltene dispersion was investigated. Since the asphaltenes were known to interact with the polar functional group such as -OH or -COOH, we conducted ring-opening reaction of the MA units of the SMA copolymer partly or fully using octadecylamine, decylamine and trioctylamine with aliphatic chains, pyridine and aniline with aromatic rings. The modification of the SMA copolymers resulted in the various polarity of the SMA copolymer. With these systematically prepared SMA dispersants, we could understand the effects of SMA polarity on the improvement of dispersibility of asphaltenes

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Non-fullerene Acceptors Materials for Polymer Solar Cells

Seung gyun Hong, Eunhee Lim*

Department of Chemistry, Kyonggi University, Korea

Bulk heterojunction (BHJ) polymer solar cells (PSCs) have been attracted due to its remarkable advantage, such as low processing cost, light weight, and semi-transparency. Generally, BHJ PSCs contain p-type organic semiconductor as donor and n-type non-fullerene semiconductor as acceptor. In the past two decades, abundant efforts have been done to develop performance of BHJ PSCs and were mainly focus on donor materials, whereas developments of acceptor materials were relatively lagged. Recently, many researchers focus on acceptor materials and shown great potential in improving the photovoltaic performance of BHJ PSCs. In order to achieve better BHJ PSCs performance, absorption spectra of donor and acceptor material should be complementary. The commonly applied methods were using narrow bandgap polymer donor to absorb long wavelength with short wavelength absorptive wide bandgap acceptor or wide bandgap polymer donor with narrow acceptor. In this study, BHJ PSCs based on narrow bandgap donor and wide bandgap acceptor materials were fabricated. The photovoltaic performance were measured and compared with component characteristics.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication and Evaluation of Porous Nano-capsule for Humidity Control

Eun Ji Park

Advanced material research division, Korea Institute of Footwear & Leather Technology, Korea

According to the National Health Statistics released by the Ministry of Health and Welfare, the average sleep time of Koreans is 6.8 hours, which is less than 7 ~ 9 hours of adult recommended sleeping time. In addition, the number of people receiving medical treatment due to sleep disorders such as insomnia is also increasing year by year. To overcome this sleep disorder, it is important to create a sleeping environment. For the smooth secretion of melatonin, a hormone that induces sleep, it is essential to secure a sleeping environment such as perfect humidity control and blocking sunlight to enable comfortable breathing. In this study, we fabricated porous nano-capsules for controlling the humidity of curtains. Also, we applied nano-capsule to fabric and evaluated absorption of humidity. The nano-capsules were characterized by FT-IR, DLS, C¹³ NMR, FE-SEM and TEM. Acknowledgement This work was financially supported by the Technology Innovation Program (10070125) through the Korea Institute for Advancement Technology(KIAT)

Poster Presentation : **POLY.P-47**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Characterization of Ultraviolet curable adhesive using urethane acrylate

Eun Ji Park

Advanced material research division, Korea Institute of Footwear & Leather Technology, Korea

In countries where security is unstable, such as countries where guns can be privately owned, are an urgent need for safety related to bulletproof. In addition to the bulletproofing applied to military facilities, there are a variety of demands for materials for bulletproofing in houses and offices used by individuals. Currently products requiring bulletproof performance are mainly used with bulletproof glass, but they have disadvantages of heavy weight due to their high specific gravity. Plastic bulletproof sheet is lighter than glass material and has excellent mechanical strength. In this study, we synthesized and evaluated ultraviolet curable urethane acrylate adhesive for use in plastic bulletproof sheet. Acknowledgement This work (S2632644) was supported by project for Cooperative R&D between Industry and Research Institute funded Korea Ministry of SMEs and Startups in 2018.

Poster Presentation : **POLY.P-48**

Polymer Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Concentration dependent excitation decays of polymer films blended with non-fullerene acceptors

Jeong Yoon Choi, Sang Woong Kang, Chan Im*

Department of Chemistry, Konkuk University, Korea

Bulk-heterojunction (BHJ) type organic solar cells have made a significant improvement by using non-fullerene acceptors to establish high power conversion efficiency. This indicates that the efficiency limits of BHJ type organic solar cells based on the electron donating polymer derivatives commonly known as P3HT or PTB7 blended with fullerene derivatives also known as PC₆₁BM or PC₇₁BM could be extended by substitution of the fullerene acceptors with novel non-fullerene type acceptors. To achieve further PCE improvement of BHJ type organic solar cells, exact understanding about exciton dissociation and recombination behaviors within BHJ thin films having various acceptor concentrations are essential. Therefore, we have performed acceptor concentration dependent transient absorption spectroscopy by using BHJ thin films consisted of typical polymer donors and non-fullerene acceptors. Those spectroscopic results are discussed in conjunction with the corresponding device performances to depict detailed behaviors of excitons as well as charge carriers within non-fullerene based active layers. This work was supported by the National Research Foundation of Korea (Project No.: NRF-2018R1D1A1B07048843 & NRF-2018K2A9A2A06023902).

Poster Presentation : **IND.P-49**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile synthesis of carbons with high micropore content as a promising adsorptive material

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Microporous carbons synthesized from sucrose and melamine in the presence of molten salts present a facile strategy to design high micropore content in the carbonaceous materials. Series of nitrogen-doped samples were prepared by changing the ratio of melamine to sucrose from 0 to 2. The optimized material possesses excellent textural features, narrow micropores and high micropore volume (



Poster Presentation : **IND.P-50**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Heteroatom-doped hierarchical porous structure as an efficient gas adsorbent

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 activation approach for designing a series of microporous carbons using economically favorable avenue. Synthesized carbon materials possess a high surface area, large pore volumes, 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-51**

Industrial Chemistry

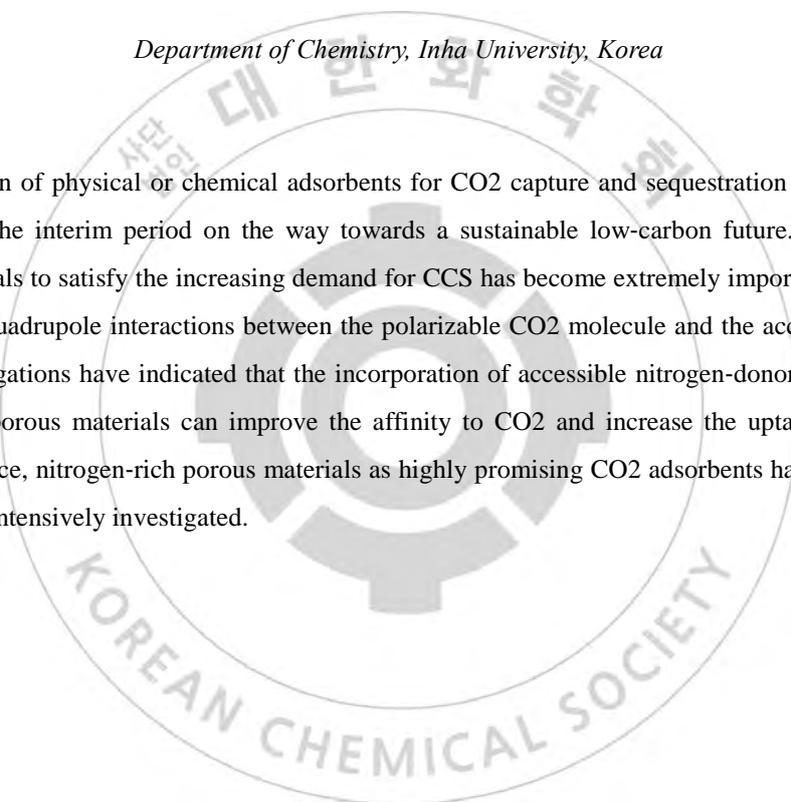
Exhibition Hall 2, FRI 11:00~12:30

Significant gas uptake by nitrogen-doped microporous carbons

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

The construction of physical or chemical adsorbents for CO₂ capture and sequestration (CCS) is a vital technology in the interim period on the way towards a sustainable low-carbon future. The search for efficient materials to satisfy the increasing demand for CCS has become extremely important. On account of the dipole–quadrupole interactions between the polarizable CO₂ molecule and the accessible nitrogen site, the investigations have indicated that the incorporation of accessible nitrogen-donor groups into the pore walls of porous materials can improve the affinity to CO₂ and increase the uptake capacity and selectivity. Hence, nitrogen-rich porous materials as highly promising CO₂ adsorbents have been broadly fabricated and intensively investigated.



Poster Presentation : **IND.P-52**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

MnO₂ and banana peel derived porous carbon composites for supercapacitors application

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, China

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-53**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode materials with high specific capacity for lithium-ion batteries

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, China

We prepared $\text{Li}_4\text{Ti}_5\text{O}_{12}$ -y solid solutions by one-step solid-state carbon thermal reduction reaction. Samples of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ -y solid solutions are synthesized with different content of carbon black. The presence of carbon black act as reductant. The formation mechanism of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ in the presence of carbon (carbon black) was investigated. Moreover, the effect of Ti^{3+} on the electrochemical performance of the $\text{Li}_4\text{Ti}_5\text{O}_{12}$ -y solid solutions has been investigated systematically. Among all samples, the sample with 2% carbon black additive exhibited the highest discharge capacity and best cycling stability. Our findings reveal that the surface modification with carbon black can improve the electrical conductivity and Li^+ diffusion coefficient and improve rate capacity and cycling stability significantly.

Poster Presentation : **IND.P-54**

Industrial Chemistry

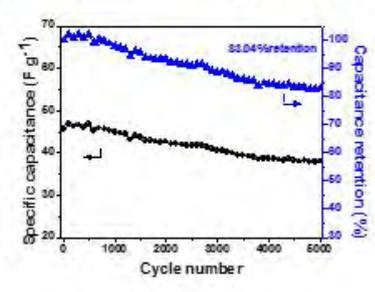
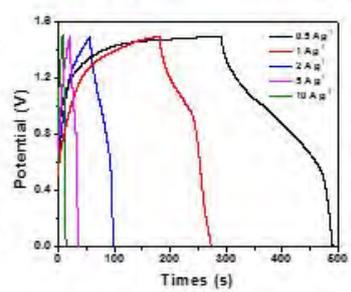
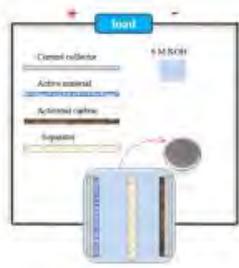
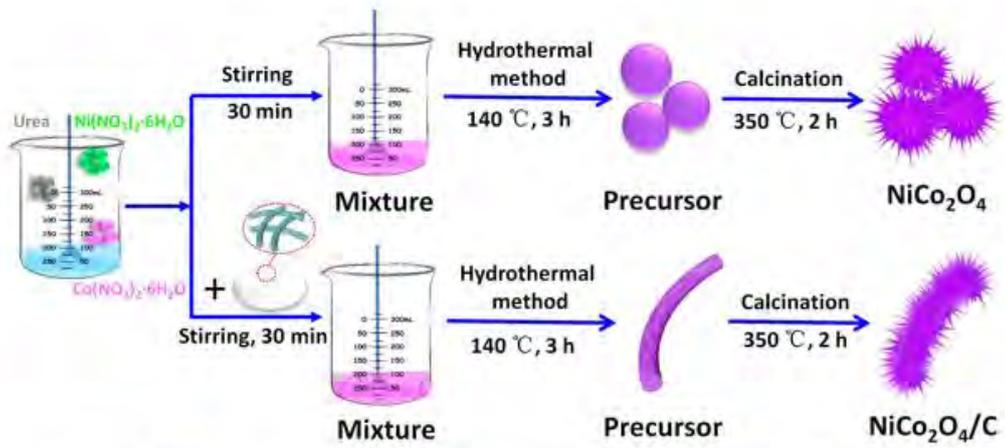
Exhibition Hall 2, FRI 11:00~12:30

Synthesis of carbon-based NiCo₂O₄ as electrodes for an asymmetric supercapacitors

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, China

We demonstrate a simple hydrothermal approach to obtain a carbon-based NiCo₂O₄ material for use in supercapacitors. In this process, filter paper was submerged in a NiCo₂O₄ precursor solution, and the final product was obtained after calcination in an Ar₂ atmosphere. The hydroxyl group-containing cellulose in the filter paper facilitates the formation of 3D structures, which not only improve the electrical conductivity but also provide fast electron and ion transport after calcination at high temperature, thus improving the electrochemical performance. An asymmetric supercapacitor has been assembled by using NCO/C-2 and activated carbon as the positive and negative electrodes. The NCO/C-2//AC ASC device exhibits 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.



Poster Presentation : **IND.P-55**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Amino functionalized graphene epoxy composites with enhanced mechanical behavior and thermal properties

Shahina Riaz, Soo-Jin Park^{1,*}

Chemistry, Inha University, Pakistan

¹*Department of Chemistry, Inha University, Korea*

Hexamethylenetetramine was used to modify GO (GO-HMTA). Influence of GO and HTMA-GO on thermal and mechanical performance of epoxy composites was studied. Commercially available diglycidyl ether of bisphenol A (DGEBA) was used as base resin. Lower loadings (0.04, 0.06, 0.08, 0.1 and 0.2 wt.%) of fillers were used to obtain the maximum improved properties. Both GO and HMTA-GO cause a sharp increase in the fracture toughness (KIC) and fracture energy (GIC) of epoxy composites at 0.04 wt.% loadings. The maximum enhancement in KIC and GIC for GO and HMTA-GO epoxy composites were 23% and 40% and 1.94 and 2.27fold, respectively. All the epoxy composites show higher integral procedural decomposition temperature (IPDT) than pristine epoxy and the maximum thermal stability of composites was obtained at 0.06 wt.% filler contents.

Poster Presentation : **IND.P-56**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile synthesis of graphene oxide-epoxy composites by thermal latent catalysts

Shahina Riaz, Soo-Jin Park^{1,*}

Chemistry, Inha University, Pakistan

¹*Department of Chemistry, Inha University, Korea*

Curing of epoxy by homopolymerization provide advantages and broadens the field of application of these polymeric materials. Cationic initiators, which remain inactive under normal environmental conditions and became active by external stimulations such as heating and photoirradiation, had been synthesized and their importance has been recognized in organic and polymer synthesis. An optimization of thermal latent cationic curing of epoxy to fabricate GO/epoxy composites with enhanced mechanical and thermal properties were carried out. Commercially available diglycidyl ether of bisphenol A (DGEBA) was used as base resin and the thermally latent catalyst, N-benzylepyrzinium hexafluoroantimonate (N-BPH) was synthesized by using the reported method. The cationic system shows excellent latent curing which was not affected by adding filler. The cure kinetics was determined by DSC measurements. An improve in the thermal and mechanical properties of composites was observed by the increment of filler contents.

Poster Presentation : **IND.P-57**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of polyethylenimine-impregnated titanate nanotubes for CO₂ capture: Influence of porosity and nitrogen content on amine-modified adsorbents

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Amine-modified adsorbents have been of interest due to their excellent performance for carbon dioxide (CO₂) capture. In this work, we have prepared titanate nanotubes (TNTs) with amine modification using polyethylenimine (PEI) for selective CO₂ capture under flue gas. TNTs were prepared by the hydrothermal reaction, and PEI-functionalized TNTs (P-TNTs) were prepared by the wet impregnation method. Enhanced CO₂ affinity through amine modification on TNTs allows for selective and favorable CO₂ adsorption onto adsorbents. To confirm the CO₂ capture in the post-combustion step, CO₂ adsorption performances were investigated by the gravimetric method under flue gas (15% CO₂ in N₂, as in fossil fuel power plants). The optimized samples with the highest CO₂ uptake (44.5 mg/g) for the CO₂/N₂ (15:85) gas mixture are attained at 313 K. This study shows that the nitrogen loading content of amine-modified adsorbents and the porosity for gas diffusion are important for practical CO₂ capture.

Poster Presentation : **IND.P-58**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Preparation and characterization 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 (H₂) 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-59**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

H₂O₂/steam activation as an eco-friendly and efficient top-down approach to enhancing porosity on carbonaceous materials : oxygen functionalities on the carbon adsorbent for CO₂ capture performance

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

The increasing concentration of carbon dioxide(CO₂) in the atmosphere is considered a major contributor to global climate changes; therefore, solid adsorbents, including porous carbon materials, have been developed as CO₂ capturing materials. Steam activation is a common method known to be effective in developing optimal micropores for CO₂ adsorption on carbon surfaces. However, it is less efficient at improving porosity compared to common chemical activation. Here, we propose an approach to improving the efficiency of steam activation in developing microporosity for CO₂ capture. In this activation, hydrogen peroxide (H₂O₂) generates the 2·OH radical in dissociation reactions at high temperatures, and a two-fold enhancement effect has been observed as compared with steam activation. However, oxygen functionalities are highly generated on carbon surfaces, which interferes with CO₂ capture performance (e.g., uptake, selectivity, adsorption rate). We used thermal reduction for removing oxygen functionalities on the carbon surface, which showed significantly enhanced CO₂ capture performance. The H₂O₂/steam activation approach could provide an opportunity for improving the textural properties of carbonaceous materials. Furthermore, our work could provide evidence that the oxygen functionalities of solid carbonaceous adsorbents influence CO₂ capture performance, including practical applications.

Poster Presentation : **IND.P-60**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

CO₂ capture with triblock copolymer activated porous carbon contained boron nitride whiskers fabricated via structure directing approach

Urooj Kamran, Soo-Jin Park*

Department of Chemistry, Inha University, Pakistan

A novel carbon contained copolymer P123 activated boron nitride whiskers (P123-CBNW) fabricated via structure directing approach. The influence of an activating agent (P123 copolymer) and melamine on adsorption efficiency of CO₂ has been reported. The maximum CO₂ uptakes tendency of prepared adsorbents was (136mg/g, 232 mg/g and 270 mg/g) at 273 K/1bar and (97 mg/g, 134 mg/g and 155 mg/g) at 298 K/1 bar for CBNW, P123-CBNW1 and P123-CBNW2 adsorbents respectively, with high isosteric heat of adsorption. Extensive analysis exposes that the presence of carbon contents, high specific surface area, high microporosity, chemically structure defects within the P123-CBNW adsorbents responsible for raising the CO₂ adsorption tendency and the selectivity over N₂ gas.

Poster Presentation : **IND.P-61**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A comparative analysis of pure and various functionalized titanate nanotubes for lithium uptakes and recovery

Urooj Kamran, Soo-Jin Park^{1,*}

Inha University, Pakistan

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In this research, the adsorption potential of lithium ions (Li⁺) by pure titanate nanotubes (TNTs) functionalized TNTs was examined. We used simple hydrothermal method for fabricating TNTs at 130 oC and these synthesized TNTs were functionalized by different OCs including urea, melamine and polyacrylonitrile using titanium (IV) oxide powder as a precursor via impregnation approach. The crystallinity, morphology and functional group properties of prepared adsorbents were characterized. The Li⁺ adsorption mechanism considered as an ion exchange reaction among Li⁺ ions and ions exist in an interlayer of pure and functionalized TNTs. Different kinetic models have applied on equilibrium experimental data to determine the rate and nature of adsorption process. The recovery of Li⁺ ions was done by using hydrochloric acid as an extracting agent with three repeated cycles. The presented study concluded that prepared adsorbents having good potential to adsorb and desorb Li⁺ ions from aqueous solution with slight reduction in capacity due to organic compounds impregnation.

Poster Presentation : **IND.P-62**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Role of P123-Copolymer in boron nitride activation for selective CO₂ adsorption

Urooj Kamran, Soo-Jin Park*

Department of Chemistry, Inha University, Pakistan

Herein, we investigated a novel carbon contained highly microporous/mesoporous copolymer P123 activated boron nitride whiskers (P123-CBNW) fabricated via structure directing approach followed by single step heat treatment under N₂ atmosphere. The influence of an activating agent (P123 copolymer) and melamine on adsorption efficiency of CO₂ has been reported. The maximum CO₂ uptakes tendency of prepared adsorbents was at 273 K, 283 K, 298 K at 1bar pressure, with high isosteric heat of adsorption. Extensive analysis exposes that the presence of carbon contents, high specific surface area, high microporosity, chemically structure defects within the P123-CBNW adsorbents responsible for raising the CO₂ adsorption tendency and the selectivity over N₂ gas.

Poster Presentation : **IND.P-63**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication of N-doped ZnO/g-C₃N₄ composites prepared by electrospinning for photocatalytic degradation of rhodamine B

SeongJun Mun, Soo-Jin Park^{1,*}

Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

Composites consisting of N-doped ZnO/g-C₃N₄ were synthesized via electrospinning and hydrothermal method. Structural properties of the composites were characterized by X-ray diffraction spectroscopy (XRD) and transmission electron microscopy (TEM). The surface areas and pore size distributions were calculated by Brunauer-Emmett-Teller (BET). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of N-doped ZnO/g-C₃N₄ composites were improved compared to pure ZnO. The results indicated that reduced g-C₃N₄ band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-64**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Pt-loaded g-C₃N₄/ZnO nanofibers for enhanced visible light photocatalytic activity via electrospinning

SeongJun Mun, Soo-Jin Park^{1,*}

Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

The Pt-loaded g-C₃N₄/ZnO nanofibers were prepared via electrospinning and hydrothermal method. The as-prepared composite photocatalysts were characterized by X-ray diffraction (XRD), Raman, scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), fourier transform infrared (FT-IR) spectra, UV-vis diffuse reflectance spectra (UV-vis DRS), Brunauer-Emmett-Teller (BET) and photoluminescence (PL). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of Pt-loaded g-C₃N₄/ZnO nanofibers were improved compared to pure ZnO. The results indicated that reduced Pt-loaded g-C₃N₄ band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-65**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of activated carbons derived from coconut shells for hydrogen storage

Ji-Hye Park, Soo-Jin Park^{1,*}

Chemistry, Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

In this work, activated carbons (ACs) were synthesized using chemical activation with various weight ratios of potassium hydroxide (KOH). The structural properties and the morphologies of ACs were investigated by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The specific surface area and pore size distribution were calculated by N₂/77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were measured by high pressure adsorption instrument at 298 K and 70 bar. The results explain that the weight ratios of carbons to KOH have an influence on the changes in pore sizes and hydrogen storage capacity.

Poster Presentation : **IND.P-66**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The influence of silica elimination on microporous carbons for H₂ uptakes

Ji-Hye Park, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, Chemical treatments of carbonized coconut shells with potassium hydroxide (KOH) were conducted for extra porosity. And then, Activated carbons (ACs) were prepared by chemical activation using KOH. The morphologies of ACs were observed by scanning electron microscopy (SEM). The structural properties were investigated by X-ray diffraction (XRD). The specific surface area and pore size distribution were calculated by N₂/77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were evaluated by high pressure adsorption instrument at 298 K and 70 bar.



Poster Presentation : **IND.P-67**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Influence of Titanium Dioxide on Photocatalytic of Polyvinylpyrrolidone based nanofibers Synthesized via Electrospinning

Yifan Zhang, Soo-Jin Park^{1,*}

Graduate School of Chemistry & Chemical Engineerin, Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

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 : **IND.P-68**

Industrial Chemistry

Exhibition Hall 2, FRI 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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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 : **IND.P-69**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

In-situ synthesis of BiOCl_x/BiOBry/BiOI_z decorated on polyacrylonitrile based nanofibers for visible-light photocatalytic investigation

Yifan Zhang, Soo-Jin Park^{1,*}

Graduate School of Chemistry & Chemical Engineerin, Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

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. Keywords: Polyacrylonitrile(PAN), Electrospinning, Photocatalytic activity, BiOCl/BiOBr/BiOI

Poster Presentation : **IND.P-70**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Oligonucleotide-Reduced Graphene Oxide Materials: Understanding Based on Electrochemical Oxidation of Guanines

Jinheung Kim

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

Investigating the interactions of biomolecules DNA/RNA with carbon nanomaterials is very important for applications in bioassay and bioanalysis. Graphene and graphene oxide (GO) have been successfully adopted by exploiting the binding affinity difference between single-stranded oligonucleotides (ssDNA) and double-stranded oligonucleotides (dsDNA) to graphene sheets. In this work, we describe the electrochemical DNA oxidation with $[\text{Ru}(\text{bpy})_3]^{2+}$ to understand the interaction between dsDNA (and corresponding ssDNA) and reduced graphene oxide (rGO). The electrochemical oxidation rate of guanine bases of ssDNA bound to rGO by electrochemically generated $[\text{Ru}(\text{bpy})_3]^{3+}$ was much slower than that unbound to rGO. Our study revealed that ssDNA constrained on rGO was significantly protected from the electron transfer to $[\text{Ru}(\text{bpy})_3]^{3+}$ because of π, π -stacking interaction between nucleobases and rGO. On the other hand, the oxidation rates of 11-, 20-, and 27-mer dsDNA bound to rGO increased relative to those of dsDNA alone, demonstrating that the guanine bases of dsDNA on interacting with rGO became more accessible to $[\text{Ru}(\text{bpy})_3]^{3+}$. Our electrochemical data illustrated that dsDNA could be totally or partially dehybridized and bind to rGO to form ssDNA/rGO. Furthermore, absorption, circular dichroism spectra, and fluorescence measurements of ethidium bromide using ssDNA and dsDNA with rGO supported the dehybridization of dsDNA in the presence of rGO.

Poster Presentation : **IND.P-71**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Home built double resonance probes for diverse non-spinning samples

Ji-Ho Jeong, 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. Many factors of each NMR 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 - ^{15}N double resonance solid-state NMR probe and a home-built 800 MHz NB ^1H - ^{15}N solid-state NMR probe for biological samples. We will also announce a home-built 400MHz and 500 MHz NB ^{19}F - ^{13}C solid-state NMR probes for analyzing nano-materials and LCD panel respectively and 600 MHz NB ^{19}F - ^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 we will introduce our recent commission task project "Development of sample dependent 400 MHz Solid-state NMR probe for the analysis of nanomaterials".

Poster Presentation : **IND.P-72**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A Detailed Raman and IR Investigation on the Satellite Vibronic Band in Blue-Emissive Pt-Complexes with High Colour Purity

Bo-Sun Yun, Su-Jin Kwak, Su-Won Na, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

We investigated the relationship between the narrowing of the emission band and structural changes using synthesized tetradentate Pt-complexes. All Pt-complexes showed phosphorescence with high color performance and the vibronic structure in the emission spectra was measured at 77 and 300 K. The 0-0 vibronic band was significantly more intense compared to the 0-1 vibronic band, due to the structural restriction of the fused tetradentate ligand. The spacing between the 0-0 and 1-0 vibronic bands were 1487 and *ca.* 1323 cm^{-1} , respectively, which were compared to the vibration modes in the IR and Raman spectra. In the transient Raman spectrum of excited **Pt-1**, the intensity enhancement and up- or down-shifting of the Raman peaks could be explained by the change of electronic distribution. Actually, the HOMO orbital was a populated Cz moiety, which shifted to the terminal-pyridine moiety represented as the LUMO. The HSOMO for the excited triplet state was delocalized on the less restricted pyrazole or imidazole moiety, as well as the pyridine moiety. Therefore, the satellite vibration bands in the emission spectra were attributed to the C=C and ring stretching of the terminal pyridine and the C-N single-bond stretching mode of Cz1-Cz2-Py.

Poster Presentation : **IND.P-73**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A Study on Polymerization Process of Polyethylene Wax with Low Molecular Weight Distribution Using Metallocene Catalysts

Minhyung Kim, Intae Kim*

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. We have evaluated hydrogen reactivity and studied on characteristics of polymerization effected by ligand structure of metallocene catalysts against Ziegler-Natta catalysts which are widely used for polymerization of polyethylene. 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). Keywords : Metallocene Catalyst, Polyethylene Wax, Polymerization Condition, Low Molecular Weight PE

Poster Presentation : **IND.P-74**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Bulkiness and Structural Isomerism of Homoleptic N-Heterocyclic Carbene Iridium(III) Complexes

Bo-Sun Yun, Jeong-Wan Yu, Jin-Hyoung Kim, Min Su Choe, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

The phosphorescence properties of ***fac*-Ir(**pmp**)₃**, ***mer*-Ir(**pmp**)₃**, ***fac*-Ir(**dmpmp**)₃** and ***mer*-Ir(**dmpmp**)₃** in CH₂Cl₂ were investigated. At 77 K, the *fac*-isomers showed blue emission with a vibronic structure, while the *mer*-isomers showed less structured emissions. At 300 K, all complexes showed broad and markedly red-shifted emission spectra compared to those at 77 K. The quantum yields of the **Ir(**dmpmp**)₃** isomers were very low, and their emission lifetimes were very short compared to those of **Ir(**pmp**)₃**. In order to understand the large differences between the photodynamic properties of **Ir(**pmp**)₃** and **Ir(**dmpmp**)₃**, we performed femtosecond time-resolved transient absorption (TA) spectroscopic measurements. The TA spectra of **Ir(**dmpmp**)₃** were almost the same as those of **Ir(**pmp**)₃** at a short delay time. However, **Ir(**dmpmp**)₃** showed a new broad TA band at around 720 nm with increasing delay time. The rise time of this band was ca. 10 ps for both isomers, and it may be attributed to the fast migration of localization of excited state via intraligand energy transfer. An electron density displacement takes place in the excited state accompany with the geometrical change of the dimethylphenyl substituent. Actually, **Ir(**dmpmp**)₃** showed a strong rigidochromic shift in the emission spectra with varying temperature. To understand the molecular orbitals and the energy levels, theoretical calculations were performed using density functional theory

Poster Presentation : **IND.P-75**

Industrial Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal-Organic Framework Database: CoRE MOF 2019

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Metal-organic frameworks (MOFs) are a class of porous crystalline materials assembled from inorganic clusters and organic building blocks. MOFs generally has high porosity, large internal surface area, and often contains active sites that can be used for site-specific adsorption and catalysis. This properties make MOFs attractive platform materials for a number of applications such as gas storage, gas separation, catalysis and chemical sensing. Recently, with tens of thousands of structures synthesized and reported, it has become increasingly important to find well-performing structures among known structures using molecular simulations. In many cases, however, the experimental structure includes solvents molecules and partially occupied or disordered atoms, which can be a significant obstacle to performing calculations. To overcome this limiting point and accelerate discovering high-performing MOFs, Chung et al. created a database called the Computation-Ready, Experimental MOF database (CoRE MOF Database 2014) derived from structures deposited in the Cambridge Structural Database (CSD). CoRE MOF Database has been used in computationally-guided screening studies and materials discovery activities, enabling researchers to discover new utility for already existing MOFs quickly. The number of MOFs reported in the literature has seen rapid growth in recent years, it is important to update database continually. In this work, we report an update of the CoRE MOF 2014 Database, including more than 15,000 structures from several different sources (contributed by CoRE MOF users, obtained from updates of the Cambridge Structural Database, and a Web of Science search). In addition, value is added to the CoRE MOF database through new analyses that can speed up future nanoporous materials discovery activities, including open metal site detection and duplicate searches. Crystal structures (only for the subset that underwent significant changes during curation), pore analytics, and physical property data are included with the publicly available CoRE MOF 2019 database.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of catalysts derived from Co & Ni containing Zeolitic-imidazolate Framework-67 (ZIF-67) and their catalytic performances for the air electrodes in Zn-air batteries

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Co & Ni embedded in the carbon nanotubes (CNT) were obtained by the calcination of Co and Ni-ZIF-67. A general and high-yield strategy for the formation of CNTs from the metal-organic frameworks (MOFs) developed at a temperature of 700 °C by the calcination process. The purpose for the formation of CNTs is to obtain small nanocatalysts with high activity. The formation of metallic Co embedded in the carbon nanotubes was investigated by the X-ray diffraction (XRD) and the graphitization was analyzed by the Raman Spectroscopy. Furthermore, the porous ZIF-67 exhibited superior electrochemical performance when applied as a cathode material for the Zn-air batteries. The cyclic test for charging and discharging was performed for 200 h revealing a potential catalyst, having splendid stability for the OER and ORR in the Zn-air batteries.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Antimicrobial activity of robust porous Cu-MOFs containing glutarates and bipyridyl ligands

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²*Institute of Nano-Bio Technology, Department of Chemistry and Nano Science, Korea*

³*Ingenium College of Liberal arts, Kwangwoon University, Korea*

Four three-dimensional (3D) Cu-MOFs formulated as $[\text{Cu}_2(\text{Glu})_2(\mu\text{-L})] \cdot x(\text{H}_2\text{O})$ (Glu is glutarate, and L is bpy = 4,4'-bipyridine (**1**), bpa = 1,2-bis(4-pyridyl)ethane (**2**), bpe = 1,2-bis(4-pyridyl)ethylene (**3**), and bpp = 1,2-bis(4-pyridyl)propane (**4**)) were synthesized by hydrothermal reactions or modified literature methods. Their crystal structures were slightly modified to increase their hydrolytic stabilities in aqueous solution. The antibacterial activities of the four Cu-MOFs, **1**, **2**, **3**, and **4**, were investigated by determining their MBC (minimal bactericidal concentration) values against five kinds of bacteria (*Escherichia coli*, *Staphylococcus aureus*, *Klebsiella pneumonia*, *Pseudomonas aeruginosa*, and *Methicillin-resistant Staphylococcus aureus (MRSA)*) which can cause water contamination, food poisoning, skin syndrome, purulent disease, pneumonia, and various diseases depending on the infection site. Although these Cu-MOFs are structurally very stable in aqueous medium during the antibacterial tests, they show excellent antibacterial activities against all five kinds of bacteria with very low MBCs. The robust porous 3D frameworks rather than the released Cu^{II} ions participate more strongly in inactivating bacteria.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Key factors determining the gas adsorption performance of zeolite granules

Ahreum Hwang

Global Technology Center, Samsung Electronics Co., Ltd., Korea

Nanoporous materials including zeolite, activated carbon, alumina, and silica have characteristics such as high surface area, high adsorption capacity, ion exchange properties and high catalytic activity, and they have been applied to various fields such as catalysis, adsorption, separation, electronics, and semiconductors. In particular, zeolite has a pore diameter of 3–10 Å, which exhibits a molecular sieving effect, and can selectively adsorb nitrogen molecules in the air using their porous structure and high surface area. However, despite the selective adsorption characteristics of zeolite, the average particle size in zeolite is in the form of a fine powder of several micrometers, and thus there are many limitations to its use as a gas adsorbent. Therefore, zeolites are often granulated by adding binders, which can improve their handling and mechanical strength. However, the addition of a binder may also decrease the adsorption performance. Therefore, we have analyzed the surface of zeolite granules, their pore size and porosity using SEM, gas adsorption, and porosimetry methods. In order to evaluate the air adsorption performance of granulated zeolite, the pressure change in the chamber of a certain volume was measured. As a result, the key factors related to the gas adsorption performance of zeolite granules were discovered. The evaluated granular zeolites have similar specific surface areas to provide gas adsorption performance, but there was a difference in their granular size and shape. In the case of zeolite I, which exhibits a large gas adsorption capacity, its pore size (300 – 400 μm) was larger than those observed for zeolite II by ~100 μm, and a large number of micropores were observed on the granulated surface. These results suggest that the surface micropores provide the primary diffusion pathway for air, which can increase the internal surface area and improve the air adsorption performance.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Structure of Cobalt(II), Copper(II) and Cadmium(II) Complexes Containing Tridentate *N,N',X*-Iminomethylpyridines

Jaegyeong Lee, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of cobalt(II), copper(II) and cadmium(II) complexes, namely $[\mathbf{L}_n\text{CoCl}_2]$, $[\mathbf{L}_n\text{CuCl}_2]$ and $[\mathbf{L}_n\text{CdBr}_2]$ supported by ligands $[\mathbf{L}_n]$ ($\mathbf{L}_n = \mathbf{L}_A$ and \mathbf{L}_B), in which $\mathbf{L}_A = (E)$ - N^1, N^1 -dimethyl- N^3 -(pyridin-2-ylmethylene)propane-1,3-diamine and $\mathbf{L}_B = (E)$ -3-methoxy- N -(pyridin-2-ylmethylene)propan-1-amine, respectively. All complexes were characterized by $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, IR, elemental analyzer and single crystal X-ray diffraction. Molecular structures of $[\mathbf{L}_A\text{CoCl}_2]$, $[\mathbf{L}_A\text{CdBr}_2]$ and $[\mathbf{L}_A\text{CuCl}_2]$ were distorted square pyramidal geometry around the metal center. The catalytic activity of the Co(II), Cu(II) and Cd(II) complexes for the methyl methacrylate (MMA) polymerization in the presence of modified methylaluminoxane (MMAO) were investigated.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Structural Characterization of [(IPMA)MX₂] (M = Co, Cu, Zn, Cd; X = Cl, Br) Supported by the ligand [IPMA]

Solhye Choe, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized and characterized a series of new cadmium(II), cobalt(II), copper(II) and zinc(II) complexes by the reaction of ligand [IPMA] where IPMA is 4-isopropyl-*N,N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)benzenamine with [CoCl₂·6H₂O], [CuCl₂·2H₂O], [ZnCl₂], and [CdBr₂·4H₂O], respectively. All complexes were characterized by IR, ¹H-NMR, ¹³C-NMR, elemental analyzer. The molecular structures of these complexes were characterized by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminumoxane (MMAO) were investigated at 60 °C.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Mixed Matrix Membranes with Porous Organic Polymers

**Dong Won Kang, Minjung Kang, Jong Hyeak Choe, Jeoung Ryul Park¹, Hyojin Kim²,
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We fabricated mixed matrix membranes (MMMs) with porous organic polymers and its inorganic acid impregnated samples. After a porous organic polymer was dispersed in DMF solution of thermoplastic polymer and the solvent was slowly evaporated, the membranes were obtained. These MMMs were characterized with infrared spectroscopy, thermogravimetric analysis, scanning electron microscope, and gas sorption. Detailed experiment contents will be explained in the presentation.

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

Inorganic Chemistry

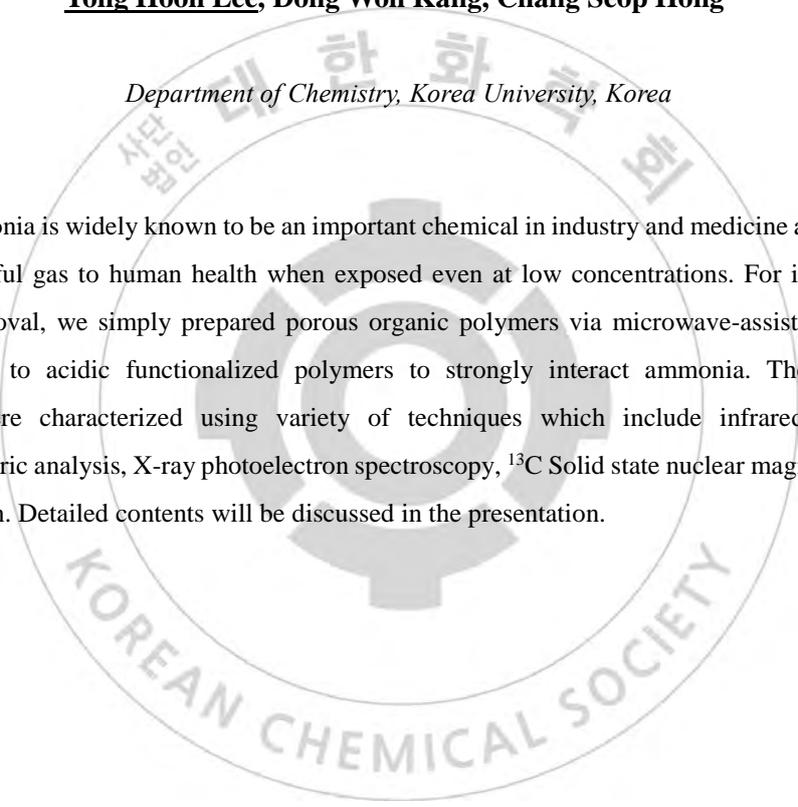
Exhibition Hall 2, THU 11:00~12:30

Postsynthetic Modified Porous Organic Polymers for Ammonia Capture

Yong Hoon Lee, Dong Won Kang, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Although ammonia is widely known to be an important chemical in industry and medicine as an ingredient, it is very harmful gas to human health when exposed even at low concentrations. For its effective and immediate removal, we simply prepared porous organic polymers via microwave-assisted reaction and modified them to acidic functionalized polymers to strongly interact ammonia. The properties of compounds were characterized using variety of techniques which include infrared spectroscopy, thermogravimetric analysis, X-ray photoelectron spectroscopy, ^{13}C Solid state nuclear magnetic resonance, and gas sorption. Detailed contents will be discussed in the presentation.



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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Quenching Responses toward Nitroaromatic Molecules in a Mn(II)-Based Metal-Organic Framework

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Metal-Organic Frameworks with π -conjugated organic linkers have attracted much attention in fluorescence sensors for specific analytes such as nitroaromatic explosives. Herein, a three-dimensional Mn-based framework $[\text{Mn}_3\text{L}_2(\text{H}_2\text{O})_3] \cdot 7.5\text{DEF} \cdot 3\text{H}_2\text{O}$ (1; H_3L = tris((4-carboxyl)phenyl)amine) was prepared by a solvothermal reaction of Mn^{2+} and H_3L in a mixed solvent of DEF/ H_2O . Mn-based framework was characterized by powder x-ray diffraction, thermogravimetric analysis, and elemental analysis. In particular, photoluminescence studies revealed that nitroaromatic explosives were fully quenched upon capture of the analytes. Detailed synthetic scheme and characterization will be presented in the poster.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

CO₂ adsorbents with improved water stability based on diamine-functionalized metal-organic frameworks

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To apply the CO₂ adsorbent to the post-combustion capture process, the materials should be water-stable because of the water vapor in the flue gas. Coating the hydrophilic polymer on the surface of the metal-organic frameworks (MOFs) helps to improve stability in an environment containing moisture. We synthesized Mn-based MOFs and functionalized with diamine to enhance the CO₂ adsorption ability and the synthesized MOF was coated with polydimethylsiloxane (PDMS) to form hydrophobic surface. The synthesized MOFs showed improved water stability in water vapor exposure test. These coated compounds were also confirmed by PXRD, infrared spectroscopy and gas sorption. Additionally, CO₂ adsorption capacity were evaluated by thermogravimetric analysis (CO₂ 15% / N₂ 85%). Detailed synthetic scheme and specific properties will be presented in the poster.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Size effect of diamine-functionalized metal-organic frameworks on carbon dioxide capture

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We controlled the particle size of Mg-MOFs with microwave_ assisted synthesis which were confirmed by scanning electron microscope. Size tuned MOFs were functionalized via post modification. X-ray diffraction, infrared spectroscopy, sorption and thermogravimetric analysis were used to elucidate properties of size tuned MOFs for carbon dioxide capture application. Detailed synthesis and properties will be presented in poster.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Time-Resolved Turn-on Fluorescence Sensing of Hydrogen Peroxide by *Ortho*-Carbazole-Appended Triarylboron Compounds

Young Hoon Lee, Heechai Lee, Juhee Kim, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

We report novel "turn-on" fluorescent probes containing a carbazolyl donor-triarylboron acceptor luminophore and dialkyl phosphine (R = Ph, *i*-Pr) as a binding site, which can efficiently monitor hydrogen peroxide (H₂O₂) in ethanolic solution. Upon addition of H₂O₂, weakly emissive phosphine compounds are changed to their phosphine oxides that can strongly exhibit green thermally activated delayed fluorescence (TADF) with microsecond-range lifetime. By using time-resolved emission techniques, the interference of the short-lived fluorescence noise can be effectively eliminated and the signal-to-noise ratio of the detecting emission can be significantly improved. Finally, the selectivity of the probes toward H₂O₂ over other analytes (e.g., various anions, biologically relevant species, and various metal ions) were also examined in EtOH at room temperature, showing high selectivity for H₂O₂.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Carbazolyl Donor-Triazine Acceptor Containing Triarylboron Compounds as Novel Fluorescent Sensors for Fluoride Anion

Heechai Lee, Hanif Mubarak, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

We report novel triarylboron-based fluorescent chemosensors for fluoride anion, *CzmBT* and *CzpBT*, where *ortho*-carbazoyl-donor and triazine-acceptor luminophores are attached to the *meta*- or *para*-position of the phenylene ring of triarylboron. To distinctly investigate fluoride binding behavior of these neutral compounds, X-ray single crystal structures of their fluoride adducts were also characterized, showing 1:1 binding between triarylboron and fluoride anion. Whereas *CzmBT* and *CzpBT* fluoresce at 561 nm and 486 nm in THF, respectively, the emission spectra are either ratiometrically changed with a gradual hypsochromic shift (*CzmBT*) or gradually quenched (*CzpBT*) upon addition of fluoride anion, allowing the detection of fluoride anion. Details of synthesis and photophysical and fluoride binding properties will be presented.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

The Chemical Crystallography Beamline with Diverse Analysis at Pohang Accelerator Laboratory

Dae-Woong Kim, Dohyun Moon*

Beam Operation Team, Pohang Accelerator Laboratory, Korea

Single crystal X-ray crystallography is very useful technique for determining the atomic or molecular structure of crystalline material. The chemical crystallography beamline is located in Pohang Accelerator Laboratory. The name of beamline is supramolecular crystallography (BL2D-SMC) that is the unique dedicated for the structure solution of crystalline materials both small and supramolecule. The beamline is located at the 2D bending magnet port in the 3GeV storage ring of Pohang Light Source II. Diffraction data are collected by a Rayonix MX225HS CCD area detector (installed in Mar. 2018). This newly installed CCD detector is performed both very fast (10 image per sec, 2x2 binned, 16 bits standard) data collection and high quality with high dynamic range (1x1 non-bin, 18 bits HDR). It will give a chance to get the structural change of the single crystals or to get the high resolution image data. The beamline control and data collection is controlled by customized BL2D-supramolecular data collection software (BL2D-SMDC). The software has an interactive GUI and is designed to run on a Windows operating system. HKL3000sm is used for cell refinement and data reduction. The instruments, status and diverse application using BL2D-SMC will be presented here.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Structural Characterization of [(PPEA)MX₂] (M = Co, Cu, X = Cl; M = Cd, X = Br) with the ligand (*E*)-2-(piperidin-1-yl)-*N*-(pyridin-2-ylmethylene)ethanamine

Seongmin Kwon, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized a series of new cobalt(II), copper(II), and cadmium(II) complexes by the reaction of ligand (*E*)-2-(piperidin-1-yl)-*N*-(pyridin-2-ylmethylene)ethanamine (PPEA). Namely, [(PPEA)MX₂] (M = Co, Cu, X = Cl; M = Cd, X = Br). These complexes were characterized by spectroscopic methods such as IR, ¹H-NMR, ¹³C-NMR and elemental analyzer. Molecular structure of [(PPEA)CuCl₂] and [(PPEA)CdBr₂] were determined by single crystal X-ray diffraction. Specifically, both complexes were a distorted square pyramidal geometry around the metal centers. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were also investigated at 60°C.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and gas sorption properties of a 3D In-MOF with diamond-like framework

Suk bin Yoon, Youngmee Kim¹, Sung-Jin Kim², Seong Huh*

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The pseudotetrahedral node, $\text{In}(\text{O}_2\text{CR})_4$, often found in In^{III} -based metal-organic frameworks (MOFs) without a cluster-based secondary building unit (SBU) is a negatively charged center due to charge mismatch between cationic In^{III} ion and four anionic carboxylate bridging linkers. Thus, In-MOFs tend to contain counter-cations near In^{III} centers in the frameworks. Dialkylammonium cations such as Me_2NH_2^+ and Et_2NH_2^+ directly derived from *N,N*-dimethylformamide (DMF) or *N,N*-diethylformamide (DEF) solvents play a significant role to form a stable framework through charge matching. If these cations thermally derived from DMF or DEF are not suitable for crystal growth of In-MOFs, it becomes very difficult to obtain high quality single crystals for structure determination. In this context, high quality crystals of In-ABDC MOF were not easily prepared from a ditopic 4,4'-azobenedicarboxylic acid (H_2ABDC) through a thermal reaction in DMF or DEF. We successfully overcome this problem by employing a room-temperature ionic liquid, 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM][BF₄]), and the resulting three-dimensional (3D) In-ABDC MOF, [EMIM][In(ABDC)₂], was structurally characterized by X-ray diffraction. The 3D framework indicates a 4-connected uninodal net with Schläfli symbol of 6^6 (dia). The gas sorption properties of solvent-free In-ABDC MOF were also investigated in detail.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Electrochemical capacitances and gas sorption properties of N-doped microporous carbon nanospheres and their KOH-activated derivatives

Hyun-Chul Kim, Minsun Park, Seong Huh*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Sub-200 nm N-doped microporous carbon nanospheres (MCNs) were directly prepared from the carbonization of as-prepared mesoporous silica nanospheres (MSNs) containing cetylpyridinium bromide (CTPB) template. After silica-etching by using HF, N-doped MCNs were obtained. The gas sorption properties and electrochemical capacitive behaviors of the N-doped MCNs were evaluated by standard volumetric method and 3-electrode measurement. The KOH-activated derivatives were also prepared for the enhancement of electrochemical supercapacitive properties. Different amounts of KOH were employed to prepare a series of KOH-activated MCNs: MCN-nKOH (n denotes the weight ratio of KOH to MCN used for activation). The N-doped MCN-nKOH series revealed superior gas uptake abilities than N-doped MCN. The N-doped MCN-2KOH sorbed $478.2 \text{ cm}^3 \text{ g}^{-1}$ ($21.33 \text{ mmol g}^{-1}$) of CO_2 at 196 K, 2.22 wt % ($11.03 \text{ mmol g}^{-1}$) of H_2 at 77 K and $162.9 \text{ cm}^3 \text{ g}^{-1}$ (7.27 mmol g^{-1}) of CH_4 at 196 K. Furthermore, the KOH-activated MCNs displayed enhanced rate capabilities of capacitance compared to the N-doped MCN. The N-doped MCN-2KOH showed the highest specific capacitance of 459.6 F g^{-1} and maximum specific energy of 37.6 Wh kg^{-1} at 0.1 A g^{-1} . It also exhibited high specific power of $53,323 \text{ W kg}^{-1}$ at 120 A g^{-1} . The N-doped MCN-nKOH materials showed very excellent electrochemical cycling stabilities up to 30,000 cycles.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Investigation of the geometric and electronic structures of the low-spin Co(IV) complex: An EPR Study

Yujeong Kim, Wonwoo Nam¹, Sun Hee Kim*

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¹*Department of Chemistry, Ewha Womans University, Korea*

High-valent metal complexes have been extensively studied for its important role of the catalytic reaction in the inorganic chemistry field. In particular, the cobalt-oxo species has been found as a reactive intermediate in several reactions, such as water oxidation, sulfoxidation reaction, and C-H activation. In this regards, the investigation of high-valent cobalt-oxo species has been highlighted in the bioinorganic, organometallic and organic chemistry fields. For several decades, a series of studies have been conducted in an attempt to mimic the biological oxidation reaction. In spite of the huge efforts, few spectroscopical studies have been carried out to suggest cobalt-oxo complexes in the bioinorganic system because of the difficulty in preparing for short-lived metal-oxo species. Herein, the studies of high-valent cobalt-oxo compounds are reported with an N₄ ligand. Multi-frequency and multi-technique EPR experiments to investigate [Co(O)L(Cl)] intermediate were performed to reveal the electronic and geometric information about the high-valent cobalt complexes. In particular, pulsed EPR techniques were performed to examine the oxo moiety with ¹⁷O labeled complex.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Operando EPR for Biomimetic Catalyst

Sugyeong Hong, Sun Hee Kim^{1,*}

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

Electron Paramagnetic Resonance (EPR) spectroscopy is a powerful tool for investigating the structure, reactivity in complex. EPR has recently become one of the important means to supplement the data obtained in the field of electrochemistry. The reason for this is that EPR analysis can identify intermediate species, identify electrochemical reaction mechanisms and reveal subtle interactions between intermediate and the surrounding environment. Due to the short life-time of intermediate species during electrochemical reaction, it is difficult to capture intermediates and the catalytic reaction is not clarified. The operando EPR is a means to complement the limit of the Ex-situ EPR. The operando EPR is a technique for measuring EPR at the same time as another reaction in progress. This approach makes it easier to overcome the limitations of the Ex-situ EPR, and furthermore to track changes in the product over the electrochemical reaction time. In this presentation, we present a new EPR cell for an essential clue to comprehend the electrochemical reaction mechanism.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Advanced Electron Paramagnetic Resonance Studies of the Manganese Nanocatalysts for Water Oxidation

Jin Kim, Sun Hee Kim*

Western Seoul Center, Korea Basic Science Institute, Korea

A tetramanganese-calcium cluster, referred to as the oxygen evolving complex (OEC), embedded in Photosystem II catalytically oxidizes water molecules to produce O₂. Inspired to the OEC, manganese oxide nanoparticles have been widely utilized to develop artificial water oxidation catalysts. Understanding characteristics of the manganese active sites is crucial to resolve the mechanism of the water oxidation and the concomitant O–O bond formation. However, the detailed information of the manganese sites at the nanoparticles, such as the local geometry and the electronic structure, has been rarely explored. In this presentation we will report the EPR (Electron Paramagnetic Resonance) analyses of the manganese oxide nanoparticles possessing catalytic activity toward water molecules. Electrochemical water oxidation mediated by the nanocatalyst was monitored by the CW EPR spectroscopy, and results revealed the change of the spin state of the manganese ions from the high-spin ($S = 5/2$) Mn(II) to the low-spin ($S = 1/2$) Mn(IV). The local geometry and the coordination modes at the particle surface could be estimated from the multi-frequency pulse EPR experiments including ENDOR (Electron-Nuclear DOuble Resonance) and ESEEM (Electron Spin-Echo Envelope Modulation) spectroscopies. Detailed characterizations of these manganese species will be discussed.

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

Inorganic Chemistry

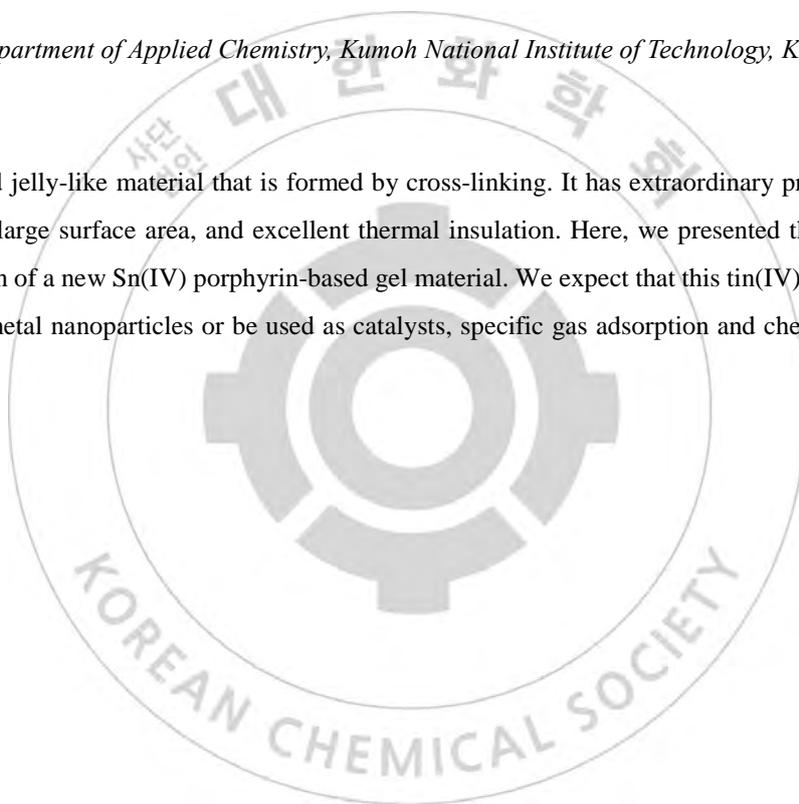
Exhibition Hall 2, THU 11:00~12:30

Preparation and Characterization of Tin(IV) porphyrin-based Gel

ChangJu Lee, Hee-Joon Kim*

Department of Applied Chemistry, Kumoh National Institute of Technology, Korea

A gel is a solid jelly-like material that is formed by cross-linking. It has extraordinary properties such as high porosity, large surface area, and excellent thermal insulation. Here, we presented the synthesis and characterization of a new Sn(IV) porphyrin-based gel material. We expect that this tin(IV)porphyrin-based gel can form metal nanoparticles or be used as catalysts, specific gas adsorption and chemical sensors in near future.



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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

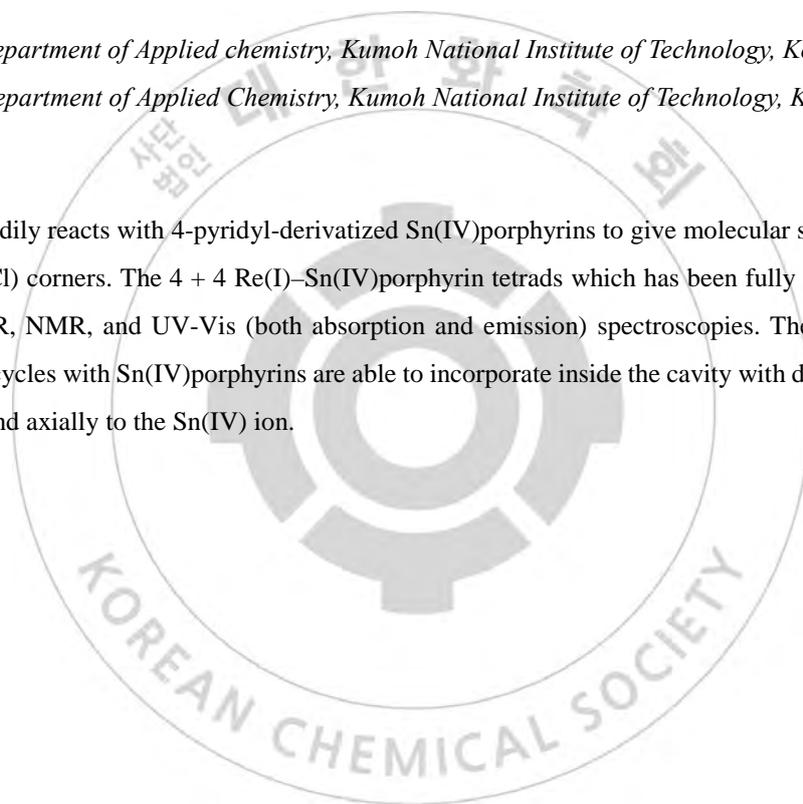
Re(I) bridged self-assembled Sn(IV)porphyrin based metallacycles

Nirmal Kumar Shee, Hee-Joon Kim^{1,*}

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Re(CO)₅Cl readily reacts with 4-pyridyl-derivatized Sn(IV)porphyrins to give molecular squares featuring fac-Re(CO)₃(Cl) corners. The 4 + 4 Re(I)–Sn(IV)porphyrin tetrads which has been fully characterized by means of FTIR, NMR, and UV-Vis (both absorption and emission) spectroscopies. The self-assembled Re(I)–metallacycles with Sn(IV)porphyrins are able to incorporate inside the cavity with different O-donor ligands that bind axially to the Sn(IV) ion.



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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Reactivity Studies of Iridium(I) Complexes of Guanidinato(1-) and Amidinato(1-) Ligands

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The reactivity of organometallic complexes with molecular oxygen is of interest because it may offer insights into how O₂ may be used to oxidize organic compounds. In reactions of alkene complexes of Ir and Rh with O₂, for example, the coordinated alkene may act as a substrate. As reported by our group previously, the use of guanidinato and amidinato ligands as supporting ligands led to the formation of (alkene)peroxo intermediates, providing insights into the mechanism of O₂ activation.^{1,2} Here, the activation of elemental sulfur (S₈) by the Ir^I alkene complexes will be described. These reactions led to the identification of multiple intermediates. Our ongoing studies are focused on the characterization of these intermediates and on understanding the mechanism of their formation.

References

- [1] M. R. Kelley, J.-U. Rohde, *Inorg. Chem.* **2013**, *52*, 2564.
- [2] M. R. Kelley, J.-U. Rohde, *Dalton Trans.* **2014**, *43*, 527.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis, Characterization and O₂ Reactivity of Ni Complexes of Redox-Active Bis(arylimino)pyridine Ligands

Jungha Lee, Jan-Uwe Rohde*

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Redox-active ligands have found increasing use in coordination chemistry because they can act as electron-reservoirs and thus expand the reactivity of the coordinated metal center. This may be advantageous, for example, for the activation of small molecules by first-row transition metals. Our group has been investigating the O₂ reactivity of bis(arylimino)pyridine radical anion complexes of Ni.¹ Here, new complexes with different substituents will be presented, with an emphasis on their characterization by electron paramagnetic resonance (EPR) spectroscopy. In addition, the O₂ reactivity of the new complexes will be described. This study provides insights into the influence of bis(arylimino)pyridine substituents on the electronic structure and the O₂ reactivity of the complexes.

References

[1] T. D. Manuel, J.-U. Rohde, *J. Am. Chem. Soc.* **2009**, *127*, 6162.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

High purity nanoparticle synthesis of core / shell structure utilizing thermal plasma technology and atomic layer deposition

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In this study, an equipment to deposit of high purity nanoparticles with core/shell structure was developed using thermal plasma technology which synthesized and deposited core material (TiO₂) on a 6-inch Si substrate to grow uniform thin film of high purity nanoparticle, and the core can be coated a shell material (Al₂O₃) without external exposure. A torch was constructed to form a stable thermal plasma which was formed by the electromagnetic waves which generated from the magnetron and propagate through the waveguide and was stabilized by the swirl gas, and a gas phase precursor was injected into the torch to deposit the core thin film. In addition, the uniformity of deposition of nanoparticles was improved by constructing a wafer holder capable of adjusting the rotation and height of the substrate. The atomic layer deposition (ALD) technique was used for shell coating of the deposited nanoparticles, and the main transfer line (MTL) was applied for transferring the substrate from the nanoparticle deposition chamber to the ALD chamber without external exposure. In addition, by constructing a pneumatic gate between the two chambers, it is possible to prevent contamination of the ALD chamber by the nanoparticles during the thermal plasma process and to maintain the vacuum state for ALD. The deposited thin film thickness of Core-TiO₂ nanoparticles and the coated shell thickness of shell-Al₂O₃ were analyzed by scanning electron microscope (SEM) and transmission electron microscope (TEM). The growth rate of core-TiO₂ thin film was 0.05 μm/s, and the coating rate of shell-Al₂O₃ was controlled with 1 Å / cycle. The crystal fraction and average particle size of core to the process conditions was analyzed through X-ray diffraction (XRD) and dynamic light scattering system (DLS), and it was confirmed that the anatase/rutile ratio of core-TiO₂ crystal structure and average core size was controlled from 0.16 to 3.16 and from 18.8 to 44.8 nm, respectively.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Effect of magnesium silicate composition and hardness on the purification ability of polyol

Jhong Ryul Yoo, HongBeom Shin, Sungho Park*

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The magnesium silicate, which is a porous material, purifies the polyol contained impurities (eg, KOH, H₂O) using adsorption, and this purification ability is evaluated in relation to the particle size and surface area of the magnesium silicate. The synthesized magnesium silicate is prepared as a powder for purification through a drying and grinding process and the particle size was changed according to hardness of dried magnesium silicate. The magnesium silicate synthesized by reacting sodium silicate solution with magnesium ion was synthesized by changing the reaction conditions such as magnesium source (MgSO₄, MgCl₂, Mg(NO₃)₂) and sodium silicate solution (No.2-Na₂O:SiO₂=1:2.7, No.3-Na₂O:SiO₂= 1:3.2). The changes of hardness and Mg / Si composition ratio according to the reaction conditions were analyzed. After drying, the hardness of magnesium silicate increased in the order of MgCl₂, MgSO₄ and Mg(NO₃)₂, and the composition ratio of magnesium silicate increased from 3.8 to 4.8 in the order of MgCl₂, MgSO₄ and Mg(NO₃)₂. That is, the higher the Si content is, the more the strength of the silicate is increased. 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. The changes of hardness and composition of magnesium silicate were not observed depending on the type of sodium silicate solution. The purification ability of magnesium silicate according to the reaction conditions was evaluated by comparing the purification ability and the purification filtration time by measuring pH change and filtration time after polyol purification.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and properties of Ni(II), Pd(II), and Pt(II) complexes with five-membered heterocyclic rings

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¹Department of Chemistry, Sungkyunkwan University, Korea

Various Pd(II) and Pt(II) complexes having five-membered heterocyclic rings were obtained from the reactions of trans-PdEt₂(PR₃)₂ or cis-PtEt₂(PR₃)₂ with organic tetrazole-thiones {S=[C{HN₄(R)}]}. Independently, treatments of Pd(N₃)₂L₂ or Ni(N₃)₂(L₂) with organic (R-N=C=S) or isocyanide (R-N≡C) afforded corresponding Pd(II) or Ni(II) complexes having heterocyclic rings or carodiimide complexes (M-N=C=N-R). The isolated complexes were determined by IR and NMR spectroscopy and X-crystallographic analyses. Experimental detail will be discussed.

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

Inorganic Chemistry

Exhibition Hall 2, THU 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 has been reported that the thermoelectric Zintl compounds $\text{Yb}_{2-x}\text{Eu}_x\text{CdSb}_2$ showed decent ZT value. However for the system, cationic mixing of Ca^{2+} and Yb^{2+} hasn't been reported. In addition, considering previously known two Zintl phases the Ca_2CdSb_2 and the Yb_2CdSb_2 compounds, $\text{Ca}^{2+}/\text{Yb}^{2+}$ cation mixing could shed a light on some interesting subjects, like structure determination by $\text{Ca}^{2+}/\text{Yb}^{2+}$ cationic ratio. Thus, a series of $\text{Ca}_{2-x}\text{Yb}_x\text{CdSb}_2$ compounds were synthesized by flux reactions, and characterized by powder and single crystal X-ray diffractions. According to SXRD refinement results, it has been observed that the compounds having relatively larger Ca content adopted the Ca_2CdSb_2 -type, while the compounds having relatively larger Yb content adopted the Yb_2CdSb_2 -type. Each structures adopt orthorhombic space group $Pnma$ for the Ca_2CdSb_2 -type and $Cmc2_1$ for the Yb_2CdSb_2 -type, and both structures are comprised of five independent atomic sites. Tight-binding linear muffin-tin orbital calculations were also performed to understand chemical bonding and the overall electronic structure. In the process, density of states and crystal orbital Hamilton population were interrogated. As a result, Ca_2CdSb_2 -type showed semiconductor behavior with narrow band gap, while Yb_2CdSb_2 -type showed poor metallic behavior with pseudogap. Currently, thermoelectric property measurements for those compounds are underway.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Eco-sustainable Fe₃ O₄ Nanoparticles Embedded Metal-Organic Framework Composite for Facile Removal of Aqueous Lead

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

Aquatic remediation using metal-organic frameworks (MOFs) has recently been proved to be an efficient technology. Designing MOFs with good stability and quick recyclable separation is still a critical challenge. Herein, a simple embedding biopolymer coated Fe₃ O₄ NPs (PFe₃O₄ NPs) in NH₂-MIL-125(Ti) was successfully demonstrated, which was further used for the efficient aquatic scavenging application. The high-resolution transmission electron microscopy (HRTEM) images illustrate that the PFe₃ O₄ NPs were uniformly embedded onto the surface of the MOF and thermogravimetric analysis (TGA) shows the high thermal stability of the composite. The composite was applied for the removal of Pb(II) from aqueous solution. The effect of various parameters like pH, contact time, initial metal ion concentration, interfering ions, and temperature on the adsorption capacity of the nanoporous composite were examined. The Langmuir model for adsorption reveals the best fitting with a maximum adsorption capacity of 561.7 mg·g⁻¹ at pH 5 and 298 K. In addition, increasing the PFe₃ O₄ precursor on nanoporous MOF decreases the recovery time (21 s), and enhances the adsorption process. The MOF composite can be recycled six times without obvious loss of the Pb(II) adsorption capacity, which is significant for its future practical use in treating industrial waste discharge and catalysis. Details of this work will be presented.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

PtM@RuO₂ nanorod (M=Ni, Co) with excellent OER activity and stability

Haneul Jin, Minki Jun, Heesu Yang, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The high cost of electricity of water electrolysis system which is induced from large overpotential is the main challenge in fulfilling the economic requirements of the viable hydrogen energy system. Developing a great catalyst for oxygen evolution reaction (OER), which is a slower half-cell reaction of water splitting, can decrease the operational cell potential. The state-of-the-art catalysts for OER are composed of a large amount of expensive iridium, however, the iridium leaching during OER operation is a serious issue to practical application. Herein, we report the synthesis of Pt embedded RuO₂ nanostructures, which are doped with transition metal (Ni or Co), namely PtM@RuO₂ (M=Ni or Co). The synthesized nanocatalysts showed great catalytic activity and stability toward water splitting reaction. We also investigated the role of embedded Pt, transition metal co-catalysts, and RuO₂ thin layer in the overall electrocatalytic OER.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Mixed metal sulfide-supported IrNi nanoparticles as extremely robust electrocatalysts for the oxygen evolution reaction

Minki Jun, Haneul Jin, Sunghyun Lim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Electrochemical water splitting is one of the sustainable and clean hydrogen production technologies. Developing active and durable electrocatalysts for enhancing the sluggish oxygen evolution reaction (OER) kinetics remains a formidable challenge. Recently, metal/metal compound heterostructures have been regarded as promising catalysts because of synergistic effects between two components. In particular, the decoration of active catalysts on a sturdy substrate can mitigate the surface deformation and migration of catalysts, which in turn greatly improve the long-term stability of the catalysts. Herein, we report the synthesis of mixed metal sulfide-supported IrNi nanoparticles as electrocatalysts for the OER. The prepared IrNi-based heterostructures exhibit superior activity and stability for the OER as compared to those of commercial Ir/C.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Highly activated hollow rhodium phosphide/sulfide: an efficient and robust electrocatalyst toward hydrogen evolution reaction

Yongju Hong, Haneul Jin, Taekyung Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The highly active and robust catalysts for the hydrogen evolution reaction (HER) are of paramount importance for the realization of hydrogen society through accelerating hydrogen production. Various transition metal phosphides, as alternative to Pt-based catalysts, with considerable catalytic performances toward HER have been reported, but their performances are still pitifully inferior to that of Pt/C. Therefore, the catalytic performance of these materials needs significant advances to replace the precious and rare Pt-based catalysts. As a method to fine-tune the surface energy states of the metal sulfide-based catalyst, the partial substitution of sulfur with phosphorous atoms has gained recent interest. Here, we synthesized rhodium-based mixed phosphosulfides by post-phosphorization of hollow rhodium sulfide and found that this anion replacement leads to a great enhancement of catalytic activity toward HER. The hollow cores and rough surface formed by the ion exchange and in-situ generated active sites seem to contribute greatly to the excellent electrocatalytic performance toward HER.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

The doping effect of transition metal in $\text{Cu}_{2-x}\text{S}@\text{IrRu}$ nanoparticles for oxygen evolution reaction in acidic media

Ye Ji Park, Jinwhan Joo, Haneul Jin, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

We have recently reported that the cactus-like $\text{Cu}_{2-x}\text{S}@\text{IrRu}$ exhibit excellent catalytic activity and stability toward the hydrogen evolution reaction and oxygen evolution reaction serving as bifunctional catalyst. It has been demonstrated in many cases that the transition metal doping to noble metal nanoparticles can greatly enhance the electrocatalytic performance of noble metal nanocatalysts. In order to develop bifunctional catalysts toward HER and OER with further enhanced catalytic activity and stability, we have attempted the transition metal doping of IrRu phase on the Cu_{2-x}S substrate. Among the tested metal dopants, Ni and Co dramatically improve electrocatalytic activity of IrRu catalyst compared to Mn and Cr. Moreover, we found that the concentration of metal dopant on the $\text{Cu}_{2-x}\text{S}@\text{IrRu}$ nanoparticles also affects the catalytic performance. Herein, we report the doping-dependent OER catalytic activity of IrRu phase as well as the reason for the observed catalytic performance.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Chiral Zinc(II) Cyclodimers: Enantio-recognition via Pulse Voltammetry

Sarada Ganguri, Ahreum Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of a series of ZnX_2 ($X^- = Cl^-, Br^-, \text{ and } I^-$) with (S)-(1-isonicotinoylpyrrolidin-2-yl)methyl isonicotinate (L) as a new chiral hemicircular bidentate ligand yields a system comprising 30-membered metallacyclodimeric species $[ZnX_2 L]_2$ with two chiral centers. In the solid state, the metallacyclodimers' packing arrays differ according to the anions and nestled solvate molecules. In the present study, the differential pulse voltammetry (DPV) technique was employed for chiral discrimination of amino acid enantiomers with S-chiral $[ZnX_2 L]_2$ and was found to be an effective tool for enantio-recognition of amino acids.



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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

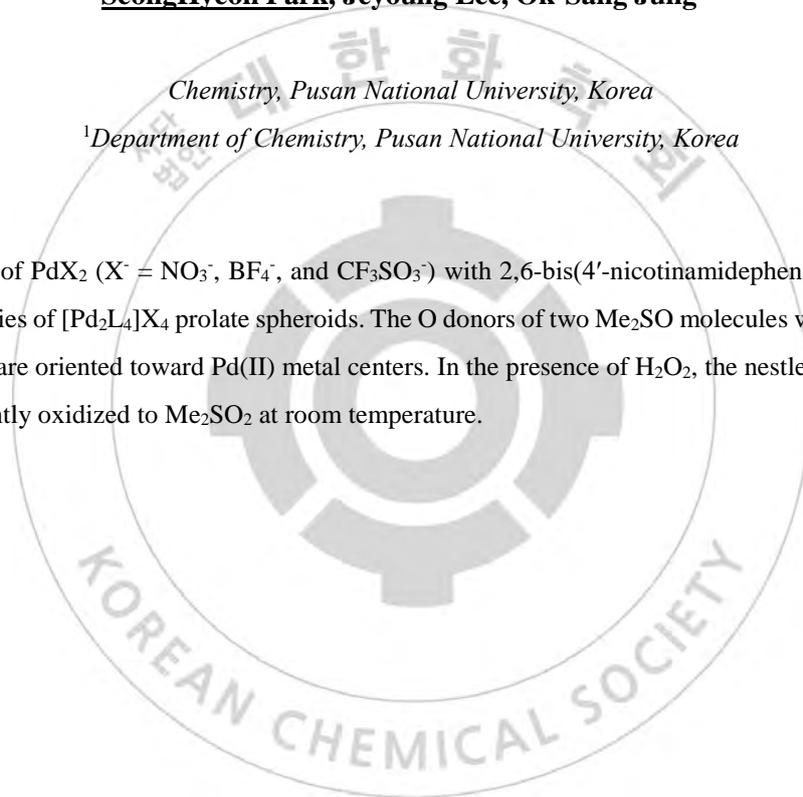
Confinement Effect of Palladium(II) cages on Oxidation via Pd₂L₄ Prolate Spheroid

SeongHyeon Park, Jeyoung Lee, Ok-Sang Jung^{1,*}

Chemistry, Pusan National University, Korea

¹*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.



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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Time-dependents self-assembly: Transformation of Kinetic into Thermodynamic Crystals

Dongwon Kim, Soojin Lee, Ok-Sang Jung^{1,*}

Pusan National University, Korea

¹*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-36**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Stable Supra Channels with Column Cyclodimeric Ensemble: Exchange and Matrix of Various Liquid Guests in SCSC Fashion

SooMin Hyun, EunSoo Yi¹, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

¹*Pusan National University, Korea*

Self-assembly of ZnI₂ with di(isoquinolin-5-yl)isophthalate (L) as a new bidentate N-donor gives rise to discrete crown-shaped M₂L₂ cyclodimers, 2CH₃CN•THF@[Zn₂I₄L₂]. These metallacyclodimers are composed of a characteristically eclipsed molecular array, resulting in the formation of unusual 10.0 x 15.1 Å² diameter suprachannels. The suprachannels adsorb/desorb various liquid molecules in a rigid manner, which enables scientists to solve the structures of various liquids. This columnar molecular ensemble is an efficient, tolerant, and reproducible suprachannel matrix for structural determination of general liquid compounds via easy single-crystal-to-single-crystal (SCSC) guest exchange without any desolvation process.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

AuAg hollow nanocubes prepared by galvanic replacement as optimized electrocatalysts for direct electrochemical CO₂ reduction

Joon Woo Park, Hyunjoon Song*

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

Since CO₂ has been pointed out as the main cause of global warming, various efforts have been put in to reduce and convert CO₂ into more useful products. Among catalysts that have been researched for CO₂ conversion, Au and Ag as electrocatalysts have been widely studied for the direct electroconversion of CO₂ to CO with high selectivity. Developing nanostructures for these noble metal catalysts are well known for their high surface area, alongside with the tunability of catalytic active sites. In this study, we present AuAg hollow nanocubes prepared from Ag nanocubes by a simple galvanic replacement reaction and their application to electrochemical CO₂ reduction catalysis. This integration of Au results in a drastic increase of catalytic surface area which leads to high mass activity and cost efficiency. Also, the overpotential for CO production is significantly enhanced compared to Ag cubes which were the template for galvanic replacement. Variations of the Au to Ag ratio are further presented to determine the optimal nanostructure and elemental composition in catalysis, and the implications on general principles for designing CO₂ reduction electrocatalysts are discussed.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Catechol Oxidation Catalysis of Bimetallic Copper (II) Cages

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 gives rise to single crystal of $[\text{Cu}_2\text{L}_2(\text{OTf})_3(\text{Sol})(\text{H}_2\text{O})_2]\text{OTf}$ (Sol = Me_2CO , H_2O , MeOH) cages. Their skeletal structure is a bimetallic cage with copper (II) (Cu(II)) sites of corresponding coordinated solvate molecules. These crystals have been employed as hetero-catalysts for 3,5-di-*tert*-butylcatechol oxidation, showing significant and different catalytic effects in dichloromethane according to the coordinated solvate molecules in the order Sol = $\text{Me}_2\text{CO} > \text{MeOH} > \text{H}_2\text{O}$. Such notable catalytic effects can be explained by the dissociation ability of coordinated solvate molecules at the catalytic center.

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

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

In-situ single-particle plasmonic imaging of electrochemical facet-selective overgrowth of Cu onto Ag nanocubes

Hyuncheol Oh, Hyunjoon Song*

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

The fabrication of bimetallic nanostructures through electrochemical methods has many advantages in catalysis and sensing due to their unique physical and chemical properties. However, it is very difficult to construct well-defined structures in the nanoscale region in this way. Herein, we investigated the facet-selective overgrowth of Cu ions onto energetically and kinetically active surfaces of silver nanocubes via spectroelectrochemistry and Matlab-coded image analysis. In a suitable chemical environment, Cu ions grow pseudomorphically in a flower-like morphology on the Ag cubes {111} surface as a function of applied potential. Nanostructuring with dendrimeric and cubic morphology is also possible by controlling only electrochemical conditions in the same chemical environment. Through our construction system and experimental conditions, a variety of Ag-Cu bimetallic nanostructures, which are very meaningful in catalysis, can be constructed. In addition, we obtained electrochemical and optical information simultaneously on growth process in real time at a single-particle level. Theoretical results of plasmon band using FDTD method provide the rationality of kinetic and mechanism analysis from correlation with experimental results. We explored the local distribution of electrochemical activities within a single nanocube, providing a great understanding on electrochemical bimetallic interconnection.

Poster Presentation : **INOR.P-40**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Diiodomethane within 1D-Ensemble Suprachannels turn into Triiodide–Iodine Channel via Photoreaction

Hyejin Oh, Sang Woo Lim, Ok-Sang Jung^{1,*}

Chemistry, Pusan National University, Korea

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

Self-assembly of ZnBr₂ with 2,7-bis(isonicotinoyloxy)naphthalene (L) yields one-dimensional (1D) zigzag chains of [ZnBr₂L] composition. This 1D chain ensemble forms unique suprachannels of 4.0 × 4.2 Å² size via weak C–H···π and π···π interactions. A 350 nm ultraviolet irradiation affects host–guest conversion. Diiodomethane molecules within the suprachannel structure of CHCl₃·CH₂I₂@[ZnBr₂L] were transformed into an unprecedented triiodide–iodine channel skeleton, HL⁺@[I₃·I₂][−]. Specifically, two clear, quasi-reversible redox peaks were observed at +0.33 and +0.70 V versus Ag/AgCl in the anodic scan and at +0.19 and +0.62 V in the cathodic scan in acetonitrile for HL⁺@[I₃·I₂][−]. **Reference** [1] Lee, H.; Hwang, S. Y.; Malenahalli H. N.; Shim, Y.-B.; Jung, O.-S. *Cryst. Growth Des.* 2018, *18*, 1956-1960.

Poster Presentation : **INOR.P-41**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of facet-controlled hollow metal-organic frameworks via cation exchange method

Sunghyun Lim, Taehyun Kwon, Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Metal-organic frameworks (MOFs) with high surface area and structural diversity have attracted a considerable interest in the research fields of gas sorption and catalysis. Cation exchange of MOFs has engendered compositionally diversified MOFs such as MOF@MOF, in which excavation of the interior can lead to a hollow MOF structure. While the number of hollow MOFs is increasing rapidly, the regiospecific metal replacement of MOFs has not been feasible. Herein, we demonstrate that shape-controlled and nano-sized MOFs can serve a suitable platform for regio-specifically composition-controlled MOFs via cation exchange, which can further invite the advent of highly complex, but well-defined hollow MOF structures. The synthetic findings of this study present a new avenue for rational design of MOFs that can be applied to important catalytic reactions.

Poster Presentation : **INOR.P-42**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis, structure and adsorption properties of Zn²⁺ and Co²⁺ based metal-organic frameworks with multifunctional ligands

Jongin Choi, Hyungphil Chun*

Department of Applied Chemistry, Hanyang University, Korea

Studies on the synthesis of metal-organic frameworks using multifunctional ligands have been carried out in different ways in expectation of various structures and properties. The functional group of the ligand is a site capable of binding to the metal, and improves the possibility that various functional groups can form various bonds and structures. 3-Amino-4-hydroxybenzoic acid contains three different functional groups, and its structure through bonding with metals is not well known. To synthesize a new structure, the metal-organic framework was combined with various metals and successfully synthesized using Zn²⁺ and Co²⁺. The structure of the new metal-organic frameworks forms a repeating structure of 8 and 4 coordination of the metal. Create a long channel through structure expansion. The gas adsorption capacity was expected in the resulting channel, but there was little adsorption to N₂ and O₂. However, it exhibited adsorption performance against H₂O and CO₂. Especially, metal-organic frameworks using Co²⁺ showed better performance than Zn²⁺

Poster Presentation : **INOR.P-43**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

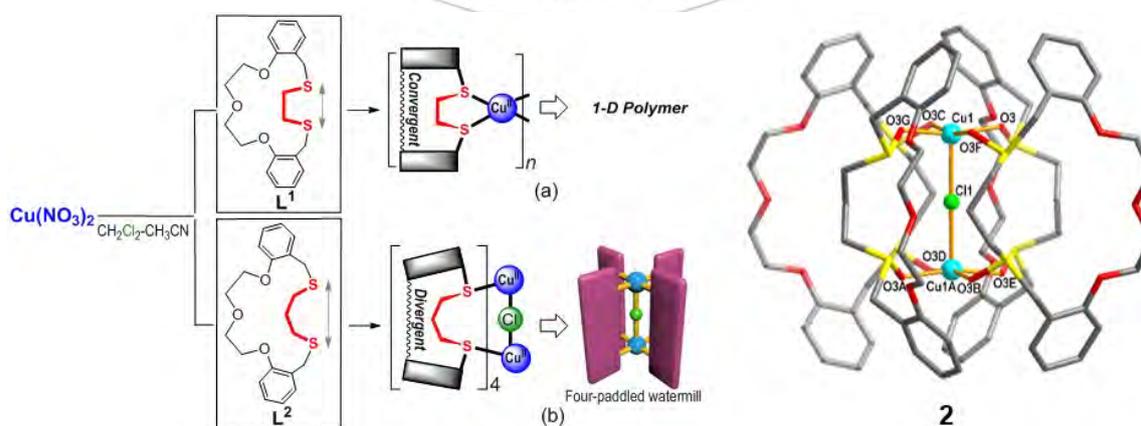
Watermill-Type Dicopper(II) Complex with Macrocyclic via Adaptive Exo-Coordination, Ligand Oxidation and Solvent Decomposition

Seulgi Kim, Han-byeol Choi, In-Hyeok Park¹, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

¹Department of Chemistry, National University of Singapore, Korea

Two O₃S₂-macrocycles with different S...S distances ($L^1 < L^2$) were employed as a strategy to isolate the adaptive products including dicopper(II) complex via controlling exo-coordination modes. L^1 gave a one-dimensional coordination polymer [Cu₂(L^1)₂(NO₃)₄]_n (**1**) based on a convergent exo-coordination. Meanwhile, L^2 resulted in the formation of a divergent exo-coordinated dicopper(II) complex [Cu₂(L^2_{ox})₄(μ -Cl)](NO₃)₄ (**2**), in which four oxidized macrocycles (L^2_{ox}) act as paddles and Cu^{II}-(μ -Cl)-Cu^{II} entity as an axis shaft adopting a four-paddled watermill. The chloro-bridging ligand (μ -Cl) in **2** is derived from the dichloromethane solvent and stabilized by C-H...Cl H-bonding. The overall watermill structure is also stabilized by interligand C-H...O H-bonding to form a pseudo-cage. The present result demonstrates that a combination of the controlled exo-coordination and the induced species serve a consistent picture of the adaptive formation of a new type dicopper(II) complex with a highly organized structure.



Poster Presentation : **INOR.P-44**

Inorganic Chemistry

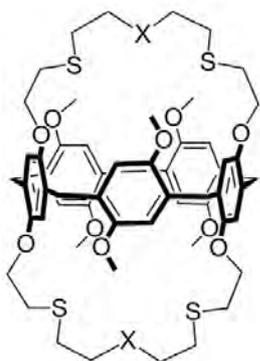
Exhibition Hall 2, THU 11:00~12:30

Adaptive Guest Binding and Coordination Networking of Pillar[5]-bis-crowns

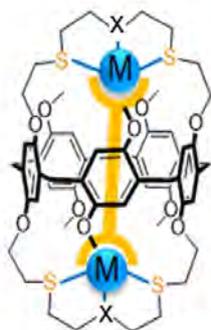
Mingyeong Shin, Shim Sung Lee*

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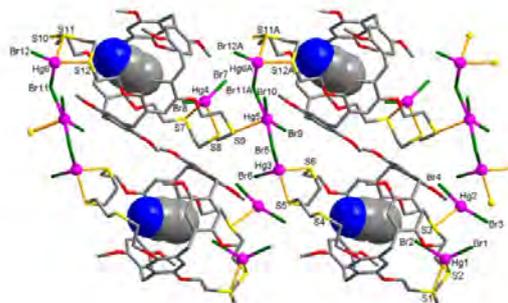
Pillar[5]-bis-crowns with different donor sets in the crown unit (L^1 : SNS and L^2 : SSS) have been synthesized and their three metallocsupramolecules (**1-3**) have been obtained. First, the assembly reactions of L^1 with silver(I) salts having different anions afforded two disilver(I) complexes $[Ag_2(L^1)(ClO_4)_2] \cdot 2CH_2Cl_2$ (**1**: perchlorate form) and $[Ag_2(L^1)(CH_3OH)_2](PF_6)_2 \cdot 2CH_2Cl_2$ (**1**: hexafluorophosphate form). In both complexes, Ag(I) center is four-coordinated by the SNS donor set in the crown unit. The observed methanol coordination to the Ag(I) center in **2** gave us an inspiration to employ some bridging ligands to replace two individual methanol molecules which bind to each metal centers. As candidates for the bridging ligands for the linking of two Ag(I) centers, dialcohols ($OH-(CH_2)_n-OH$), dinitriles ($CN-(CH_2)_n-CN$), and dicarboxylates ($-OOC-(CH_2)_n-COO-$) are expected to show a length-selective recognition behavior depending on the values of n (1, 2, or 3..). These results might be a chemical example of the adaptive guest binding which observed in biology. Next, L^2 reacts with $HgBr_2$ to give a 1-D coordination polymer $[Hg_6Br_{12}(CH_3CN@L^2)_2]_n$ (**3**) in which two L^2 ligands up and down are linked by a linear Hg_3Br_6 unit to form a C-type dimer and the adjacent dimers are further linked by Hg-S bonds, giving rise a unique 1-D ribbon type structure with a poly(dimer) connectivity pattern.



X = NH ; L¹
X = S ; L²



= dialcohols, dinitriles
Or dicarboxylates



3, [Hg₆Br₁₂(CH₃CN@L²)₂]_n



Poster Presentation : **INOR.P-45**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Hierarchically branched trimetallic nanocage as a highly active and durable electrocatalyst toward the methanol oxidation reaction

Seokpyo Jeon, Songa Choi, Ye Ji Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Pt-based nanomaterials are well-known for catalyzing methanol oxidation reaction (MOR) in the anode of DMFCs. However, high cost, low abundance, and CO poisoning of Pt-based catalysts impede the practical use of DMFCs. Therefore, fabrication of economical Pt-based alloy catalysts toward the MOR has been intensively investigated. Among the possible approaches, trimetallic nanostructures have received great interests due to their unprecedented synergistic effect among multiple components on the surfaces. Recently, hollow- and cage-like nanostructures have been explored in order to achieve large Pt dispersion on their active surface sites. In this work, we combined these activity-boosting strategies to build Ru branched RuPtCu ternary alloy nanocage as a promising MOR catalyst. Electrochemical MOR activity and stability of the Ru branched RuPtCu nanocages are greatly promoted compared to those of PtCu and RuPtCu nanocages and the state-of-the-art Pt/C. We expect that this synthetic methodology will pave the way for further development of multicomponent nanoframe catalysts toward important electrocatalytic processes.

Poster Presentation : **INOR.P-46**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Ni₃S₂ Octahedral Nanocage as an Efficient Electrocatalyst for Hydrogen Evolution Reaction

Jinhyoung Jo, Jun Kim, Taekyung Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

While the continuous consumption of fossil fuels has alarmed the world with innumerable environmental issues, the demand for clean energy sources in the near future is ever increasing. To realize hydrogen economy, water electrolysis is considered one of the most promising solutions, and development of efficient electrocatalysts is expected to accelerate the commercialization of water electrolysis. The best known electrocatalyst for hydrogen evolution reaction (HER) is platinum, however, due to its scarcity in the earth crust, many researchers are focusing on discovering non-noble metal-based materials. As noble metal alternatives, metal phosphides and sulfides have been investigated with a great fervor. Among them, Ni₃S₂ phase has shown a great promise as HER catalyst. However, this phase has never been synthesized by solution-based synthetic approach. Herein, we report the first solution-based synthesis of Ni₃S₂ octahedral nanocage (ONC), which is an efficient electrocatalyst for HER.

Poster Presentation : **INOR.P-47**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

One-pot synthesis of composition-tunable core-shell ternary nanowires and their composition dependent activity toward the oxygen evolution reaction

Heesu Yang, Taehyun Kwon, Jinwhan Joo, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

With the increasing demand for sustainable energy sources, water splitting technology has become one of the promising routes to overcome environmental issues. Among various nanostructured catalysts, 1-D nanostructures of precious metals established themselves as promising electrocatalyst due to their multiple anchoring points among themselves ensuring the thermal stability. On the other hand, core-shell nanoparticles with lattice mismatch between the core and the shell are used to render high surface energy that enhances catalytic activity. We have strived to form 1-D nanocatalysts with core-shell structure to benefit from both features of 1-D nanostructure and core-shell. In this work, we report the synthesis of core-shell nanowire with composition-tunable core by one-pot synthesis, which showed that the electrocatalytic activity toward oxygen evolution reaction (OER) varies in accordance with core-composition.

Poster Presentation : **INOR.P-48**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Heterophase Ir/Pt nanoframes as efficient electrocatalysts toward oxygen evolution reaction

Songa Choi, Seokpyo Jeon, Ye Ji Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

IrO_x and RuO_x have proven to be the most active electrocatalysts for oxygen evolution reaction (OER). However, the IrO_x and RuO_x based nanoparticles agglomerate with higher ohmic resistance to hinder the electronic paths and lower their stability. We posited that the design of Pt/IrO₂ catalysts might be beneficial because the Pt phase can increase the electronic conductivity. Herein, we report the synthesis of heterophase IrNi/PtNi nanoframe by controlling the differences in decomposition kinetics of each metal precursor and gas type between argon and carbon monoxide. The Ir oxide phase, obtained from electrochemical oxidation, on the metallic PtNi phase efficiently catalyzed the OER in acidic media

Poster Presentation : **INOR.P-49**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Iridium Cobalt Alloy Nanoparticles on Co_xS_y Nanocage as a Robust Bifunctional Electrocatalyst in Water Splitting Catalysis

Jun Kim, Jinwhan Joo, Jinhyoung Jo, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The development of cost-effective electrocatalysts is critical in practical water electrolysis. While precious metal-based nanomaterials are strong candidates as catalysts due to their favorable intrinsic properties for hydrogen and oxygen evolution reaction (HER and OER), however, the issues of low natural abundance always remain for these materials. Furthermore, along with the cost issue, the long term stability of catalysts is indispensable requirement for practical application. In particular, while iridium-based nanoparticles have shown excellent initial catalytic performances toward OER, they have not shown acceptable level of long-term stability for practical application. In order to boost the catalyst stability, we have deposited iridium cobalt alloy on an inert Co_xS_y nanocage that deters the surface migration of iridium oxide phase during catalysis. Herein, we report iridium cobalt alloy on Co_xS_y nanocage as a bifunctional electrocatalysts for efficient water splitting catalysis.

Poster Presentation : **INOR.P-50**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Transition metal oxide/chalcogenide arrays on nickel foam for efficient and stable electrocatalysts

Jinwhan Joo, Jun Kim, Taekyung Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The development of highly efficient and stable electrocatalysts for water splitting at large current density is necessary for hydrogen industry, however, the road to full implementation of the water splitting technology is full of obstacles. Recently, directly grown catalysts on nickel foam have attracted enormous attention and effort, due to their low overpotential and large current density. Herein, we report the preparation of novel nanostructured transition metal oxide/chalcogenide arrays on nickel foam that show high catalytic activity and stability for water splitting. Owing to the synergistic effect at the hetero-interface, a superior electrocatalytic performance at large current density could be achieved.

Poster Presentation : **INOR.P-51**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of 3d transition metal-doped PtZn intermetallic nanoparticles by using ZIF-8 nanocubes as a template

Taehyun Kwon, Doyeop Kim, Sunghyun Lim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nanoparticles with structurally ordered alloy phase have received a great attention due to their higher catalytic activity and stability than random alloy phase. Many studies have been carried out to prepare and control the crystal structure of intermetallic nanoparticles, however the examples of intermetallic alloy nanoparticles are limited to only a few phases. Furthermore, unlike random alloy case, it is very difficult to introduce the hetero-atoms as a dopant to the intermetallic phase. We have successfully introduced 3d-transition metal dopants with controlled amounts to ZIF-8 nanocubes by one-pot process. Moreover, the 3d transition metal-doped ZIF-8 nanocubes were further transformed into 3d transition metal-doped PtZn intermetallic nanoparticles via Pt²⁺ cation exchange and thermal annealing process.

Poster Presentation : **INOR.P-52**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design and Synthesis of Ruthenium Aqua Complexes Featuring Oxidation Potential Inversion 1

Byung Wook Lee, Young Hoon Jang, Youn Kyung Kang*

Department of Chemistry, Sangmyung University, Korea

The DFT calculation protocols that are able to predict potential inversion behavior of Ru-aqua complexes have been recently established (PBE1PBE/def2SVP/SDD; protocol A and mPW1LYP/6-31g(d)/LANL2DZ; protocol B). For the rational design of series Ru complexes that exhibit potential inversion during the sequential two-electron proton-coupled oxidations, Ru-OH₂→Ru=O via Ru-OH state, we performed DFT calculations by employing protocols A and B over 50 mononuclear Ru complexes. A number of [Ru(DAMP)(BIAN)(H₂O)]²⁺ complexes, where DAMP=2,6-bis(dimethylaminomethyl)pyridine and BIAN=bis(arylimino)acenaphthene, were selected as appropriate candidates and synthesized. Systematic evaluation of ligand electronic effects on the potential inversion behavior was performed. Experimental electrochemical data were compared with the DFT results and the major factors that govern the proton-coupled oxidation potentials were interrogated. These experiments provided useful design motif of Ru-aqua complexes for the development of future water-oxidation catalysts.

Poster Presentation : **INOR.P-53**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Organic mixed-valence system: Rigid, cofacially compressed, π -stacked organic compound with phenylene spacer(s) and naphthalene pillar(s).

Hae Won Jung, Youn Kyung Kang*

Department of Chemistry, Sangmyung University, Korea

Distance dependence of electronic coupling matrix element is a key to identify the charge mobility of the medium. Given the intense interest toward the high charge mobility organic materials, information regarding the distance dependence of electronic couplings for the π -stacked aromatic scaffold is of great importance. Here we provide such information from the study of series mixed valence systems : anion radical $[Q-(ph)_n-Q]^-$ and cation radical $[D-(ph)_n-D]^+$ systems where Q = 2,5-benzoquinone, D= 2,5-dimethoxybenzene, ph = phenyl, and n = 0, 1 and 2. Electronic couplings were experimentally determined by the spectroelectrochemical method that gave distinct charge transfer bands by electrochemical reduction ($[Q-(ph)_n-Q]$ to $[Q-(ph)_n-Q]^-$) or oxidation ($[D-(ph)_n-D]$ to $[D-(ph)_n-D]^+$). Mulliken-Hush relation was used to extract electronic coupling values. Decay parameters(β) of distance dependences of $[Q-(ph)_n-Q]^-$ and $[D-(ph)_n-D]^+$ series were found to be very mild (< 0.3) implying that simple aromatic building blocks can provide substantial D-A electronic coupling when organized within a π -stacked structural motif with a modest degree of arene-arene interplanar compression.

Poster Presentation : **INOR.P-54**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design and Synthesis of Ruthenium Aqua Complexes Featuring Oxidation Potential Inversion 2

Young Hoon Jang, Byung Wook Lee, Youn Kyung Kang*

Department of Chemistry, Sangmyung University, Korea

The DFT calculation protocols that are able to predict potential inversion behavior of Ru-aqua complexes have been recently established (PBE1PBE/def2SVP/SDD; protocol A and mPW1LYP/6-31g(d)/LANL2DZ; protocol B). For the rational design of series Ru complexes that exhibit potential inversion during the sequential two-electron proton-coupled oxidations, Ru-OH₂→Ru=O via Ru-OH state, we performed DFT calculations by employing protocols A and B over 50 mononuclear Ru complexes. A number of [Ru(PIMP)(BIAN)(H₂O)]²⁺ complexes, where PIMP=2,6-bis(2,4,6-trimethylphenyliminomethyl)pyridine and BIAN=bis(arylimino)acenaphthene, were selected as appropriate candidates and synthesized. Systematic evaluation of ligand electronic effects on the potential inversion behavior was performed. Experimental electrochemical data were compared with the DFT results and the major factors that govern the proton-coupled oxidation potentials were interrogated. These experiments provided useful design motif of Ru-aqua complexes for the development of future water-oxidation catalysts.

Poster Presentation : **INOR.P-55**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Nanoparticle anisotropy control via surface energy modulation

Taekyung Kim, Yongju Hong, Jun Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Multiphasic nanocrystals with hetero-interfaces are interesting because they can possess interesting physicochemical properties. In particular, solid-solid interfaces are important in controlling the activities of electrocatalysts because 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 multiphasic nanostructures. Cation exchange reactions are useful tools in inducing phase transformations in nanoparticles. When one type of cations exchanged by other cations, a new phase is produced and thus the heterogeneous interfaces are formed. In this research, we report the synthesis of the colloidal hybrid nanoparticles having solid-solid interfaces based on copper sulfide templates and unusual atom migration on the nanoparticle surface depending on the surface energy of the nanocrystals.

Poster Presentation : **INOR.P-56**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Well-Arranged and Confined Incorporation of PdCo Nanoparticles within a Hollow and Porous Metal-Organic Framework and Its Superior Catalytic Activity

Sojin Oh, Jian Yeo, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The catalytic activity of metal nanocatalysts generally decreases due to the agglomeration of unstable nanocatalysts during the catalytic reaction. Therefore, the well-arranged incorporation of catalytically-active metal nanoparticles within porous materials is very important to preserve their original activity by preventing the agglomeration of unstable nanocatalysts. Herein, we present a convenient method for the well-arranged incorporation of bimetallic PdCo nanocatalysts within unique hollow and porous carbon material or metal-organic framework (MOF) support. Several chemical conversions occur simultaneously during one-step low temperature pyrolysis of polystyrene@ZIF-67/Pd²⁺ core-shell microspheres [where ZIF (zeolitic imidazolate framework) is a subclass of MOF]: the polystyrene core within a core-shell microsphere is removed, and so resulting in a hollow support; the ZIF-67 shell acts as a well-defined porous support and also as an appropriate Co²⁺ supplier for the formation of metal nanocatalysts; and Pd²⁺ and Co²⁺ are reduced to form catalytically-active bimetallic PdCo nanoparticles. The resulting composites show a superior catalytic activity owing to the unique hollow and porous features of support and the well-arranged incorporation of highly-active bimetallic PdCo nanoparticles within a unique hollow and porous support.

Poster Presentation : **INOR.P-57**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Co- and N-codoped Porous Carbon Catalyst Made from Core–Shell Type Hybrid MOF (ZIF-L@ZIF-67) and Its Efficient Oxygen Reduction Reaction (ORR) Activity

Sujeong Lee, Sojin Oh, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The development of carbon-based oxygen reduction reaction (ORR) catalysts to replace the expensive and unstable platinum-based ORR catalysts is of great importance for their optimal utilization in energy conversion and storage. Herein, we present the production of highly active carbon-based ORR catalyst from well-designed core–shell type hybrid metal–organic framework (MOF). Cobalt- and nitrogen-codoped porous carbon leaves (Co,N-PCLs) are prepared via a simple one-step pyrolysis of well-designed leaf-shaped core-shell type hybrid MOFs [ZIF-L@ZIF-67, ZIF (zeolitic imidazolate framework) is a subclass of MOF], which contain two different metal ions (Zn^{2+} in core and Co^{2+} in shell) and sufficient nitrogen source with a thin flat morphology. Owing to their unique structural and compositional features, Co,N-PCLs display much better ORR activity than their counterparts prepared from the parent materials (ZIF-L or ZIF-67). In addition, Co,N-PCLs even show a better electrochemical stability and a better methanol tolerance compared to commercial Pt/C material.

Poster Presentation : **INOR.P-58**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Unbalanced MOF-on-MOF Growth for Production of Lopsided Core-Shell of MIL-88B@MIL-88A with Mismatched Cell Parameters

Dooyoung Kim, Gihyun Lee, Sojin Oh, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The integration of two MOFs with matched cell parameters is frequently performed, and results in the isotropic growth of the second MOF. However, MOF-on-MOF growth with mismatched cell parameters is more challenging, and typically results in the anisotropic growth of the second MOF on the template MOF. Herein, we demonstrate the formation of an atypical lopsided core-shell of MIL-88B@MIL-88A via unbalanced MOF-on-MOF growth. Despite the large overall mismatch in the cell parameters of MIL-88A and MIL-88B due to the incorporation of different organic linkers (1,4-benzenedicarboxylic acid and fumaric acid, respectively), the similarity in the ab plane within the core and shell enables abnormal anisotropic MOF-on-MOF growth. The formation mechanism of the lopsided core-shell was verified by monitoring the samples at different time points by electron microscopy analyses.

Poster Presentation : **INOR.P-59**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Metal doped Ru oxide-based nanocrystals toward efficient water splitting reaction

Songa Choi, Intaek Yeo, Yongju Hong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

RuO_x based nanocrystals, which is used as oxygen evolution reaction (OER) catalysts, have a very high intrinsic OER activity in acidic media and are less expensive than more extensively studied IrO_x catalysts. However, the instability of RuO_x phase has posed as a formidable barrier for the practical application of the RuO_x-based nanocatalysts. Recently, we have demonstrated that noble metal Pt doping of RuO_x phase can greatly improve both the activity and stability. Herein, we demonstrate that the alloy composition of PtCo can further improve the activity and stability of RuO_x phase for the OER. We also report the role of dopants in the active and stable catalysts examined by various analytical tools.



Poster Presentation : **INOR.P-60**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

New platform to Measure Thermopower of Molecules: Eutectic Gallium-Indium Electrode based Large-area Thermoelectric Junctions

Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

An important goal in molecular thermoelectrics is to establish atomic-detailed structure-property relationship. To achieve this goal, a reliable and reproducible platform relevant to molecular-level thermoelectric measurements is essentially needed. In this presentation, we show a new, efficient approach for thermoelectric characterization of large-area of molecular monolayers using cone-shaped liquid eutectic gallium-indium alloy (EGaIn). Our method enables non-invasive, reversible top-contact over delicate organic surfaces in ambient conditions and high yields of working devices (up to 97%). Thus, we can obtain statistically sufficient thermoelectric data sets (~6000 data per sample in a few hours). We estimate for the first time Seebeck coefficient values of EGaIn ($3.4 \pm 0.1 \mu\text{V/K}$) and the Ga₂O₃ layer ($3.4 \pm 0.2 \mu\text{V/K}$) on the EGaIn conical tip. With widely studied molecules, oligophenylenethiolates, we further validate the newly developed large-area thermoelectric junction platform.

Poster Presentation : **INOR.P-61**

Inorganic Chemistry

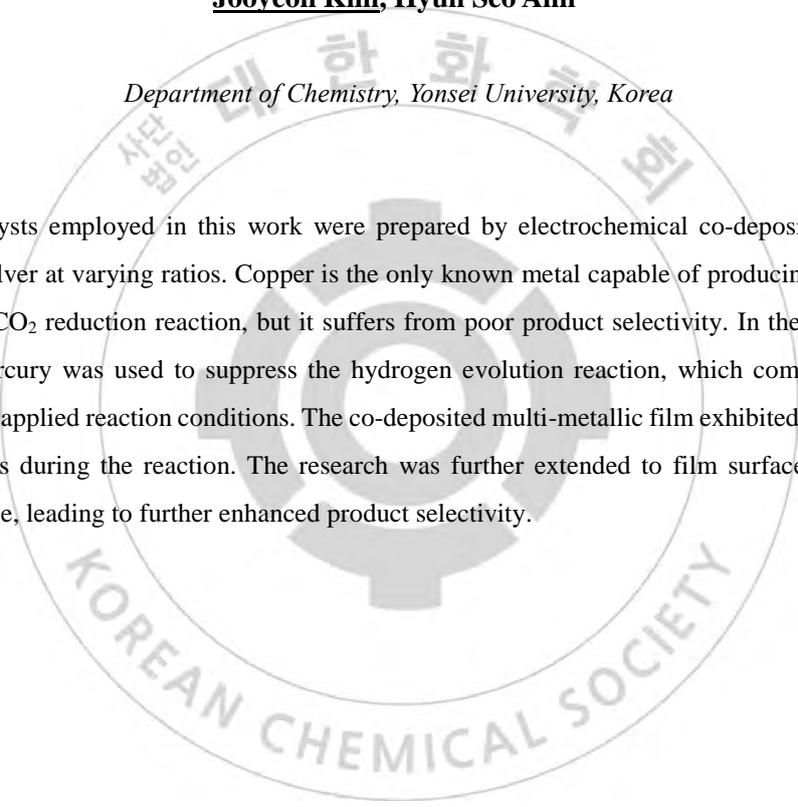
Exhibition Hall 2, THU 11:00~12:30

Mechanochemically Exposed Cu-Ag-Hg Multi-Metallic Thin Films for Improved CO₂ Reduction Electrocatalysis

Jooyeon Kim, Hyun Seo Ahn*

Department of Chemistry, Yonsei University, Korea

Thin film catalysts employed in this work were prepared by electrochemical co-deposition of copper, mercury, and silver at varying ratios. Copper is the only known metal capable of producing hydrocarbons as products of CO₂ reduction reaction, but it suffers from poor product selectivity. In the study, the film doped with mercury was used to suppress the hydrogen evolution reaction, which competes with CO₂ reduction in the applied reaction conditions. The co-deposited multi-metallic film exhibited high selectivity for C₂₊ products during the reaction. The research was further extended to film surface fabrication by mechanical force, leading to further enhanced product selectivity.



Poster Presentation : **INOR.P-62**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Chemical Strategies to Modify Amyloidogenic Peptides by Iridium(III) Complexes: Coordination and Photo-Induced Oxidation

Juhye Kang, Jung Seung Nam, Tae-Hyuk Kwon¹, Mi Hee Lim^{2,*}

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

¹*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

²*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Amyloidogenic peptides are considered central pathological contributors towards neurodegeneration as observed in neurodegenerative disorders [e.g., amyloid- β ($A\beta$) peptides in Alzheimer's disease (AD)]; however, their roles in the pathologies of the diseases have not been fully elucidated since they are a challenging target to be studied due to their heterogeneous nature and intrinsically disordered structure. Chemical approaches to modify amyloidogenic peptides would be valuable in advancing our molecular-level understanding of their involvement in neurodegeneration. In this presentation, effective chemical strategies for modifications of $A\beta$ peptides implemented by a single Ir(III) complex in a photo-dependent manner will be presented and discussed. Such peptide variations can be achieved by our rationally designed Ir(III) complexes leading to the significant modulation of the aggregation pathways of $A\beta_{40}$ and $A\beta_{42}$, as well as the production of toxic $A\beta$ species. Overall, we demonstrate chemical tactics for modifications of amyloidogenic peptides in an effective and manageable manner utilizing the coordination capacities and photophysical properties of transition metal complexes.

Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Sr-glass to capture CO₂ coming from the treatment of carbowastes

Hyung-Ju Kim

Korea Atomic Energy Research Institute, Korea

There are several different carbowastes coming from nuclear power plant (NPP) containing ¹⁴C such as spent activated carbon, spent resin, and irradiated graphite etc. Each NPP generates hundreds of carbowastes every year. Since deposited amount of carbowaste causes significantly demanding disposal cost as well as stability issues, it is necessary to reduce the quantity of wastes. Spent activated carbon comes from HVAC (heating, ventilation, and air conditioning), and it is used for the adsorption of I to protect radiation worker. Resin is used for ion exchange material to remove gamma nuclides. The graphite is irradiated when it works as moderator. In the process of their role, the ¹²C in the materials is converted to the ¹⁴C. Thus, ¹⁴C is the major issue to be removed for safe disposal. CO₂ capture using adsorbents is under research by using a number of novel materials to improve their performance. Inorganic materials are advantageous due to its high stability and ease of surface modification. To safely treat the ¹⁴C, CO₂ capture can be used. Moreover, final form of CO₂ must be considered to further solidify the product. Here, we present CO₂ capture using Sr-incorporated glass. This adsorbent has large amount of Sr to sequester CO₂, and strontium carbonate as product is preferred form for solidification. The resulting Sr-glass exhibits high CO₂ capacity (>2.5 mmol CO₂/g adsorbent) in aqueous stream under mild conditions. To optimize the CO₂ capture capacity, we performed CO₂ capture with different conditions to increase CO₂ capacity upto 4.0 mmol CO₂/ g adsorbent.

Poster Presentation : **INOR.P-64**

Inorganic Chemistry

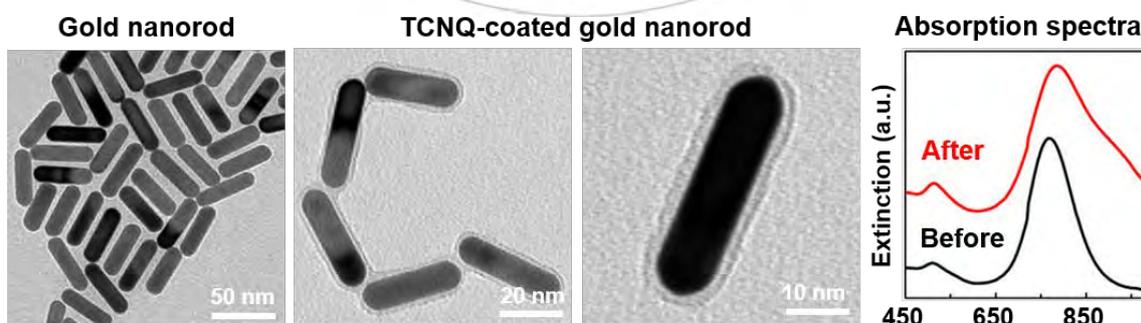
Exhibition Hall 2, THU 11:00~12:30

Redox-active π -stacking molecule coating on gold nanorods

Jaedeok Lee, Hyoseong Lee, Juyeong Kim*

*Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University,
Korea*

Current electronic device fabrication is pushed by a continual demand for smaller and faster processing units. Constructing electronic devices from nano-sized building blocks promises a solution. Engineering self-assembly of colloidal nanoparticles is recognized as a likely stream to fabricate next generation devices. However, there are still challenges to make colloidal nanoparticle-based devices as comparable as and even beyond conventional ones such as overcoming limit in charge transport between nanoparticles. We use tetracyanoquinomethane (TCNQ), known as redox-active, to coat the gold nanorod surface, aiming at facilitating the charge transport between assembled gold nanorods. After the reaction between aqueous gold nanorods and TCNQ molecules, we observed by transmission electron microscopy a thick shell layer was formed on the nanorod surface. The shell formation was investigated further with different reaction parameters (reaction time, stirring rate, aging time of the TCNQ solution), and its reaction mechanism could be derived.



Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Aluminum Complexes Containing Phenoxyimine Ligands and Their Application into CO₂ Conversion

SeungYeon Cho, Youngjo Kim*

Department of Chemistry, Chungbuk National University, Korea

Research on organometallic catalysts for the efficient synthesis of cyclic carbonates from epoxides and Among the chemical transformation of CO₂, the synthesis and application of cyclic carbonates made from the cycloaddition of carbon dioxide and epoxide is the most active research area. In order to efficiently synthesize CO₂-based cyclic carbonates, metal-based catalysts are required. Especially, the most common metal center for these catalysts is aluminum, because Al is present in the clust and is environmentally friendly. In this study, we will report the synthesis of new aluminum-based catalysts containing substituted phenoxyimine ligands with different electron density and their application as catalysts for the cycloaddition of CO₂ and epoxides under the various conditions.

Poster Presentation : **INOR.P-66**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Ruthenium(III) Nitrosyl Complexes Containing bis-Carboxamide Tetradentate Ligand: Syntheses, Structures and Photoreactivities

Jang hoon Cho, Manho Lim¹, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

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

Nitric oxide plays an important role in many biological signaling processes including blood pressure regulation, neurotransmission, inflammatory response, and programmed cell death. For the purpose of controlling the physiological processes, compounds that selectively release nitric oxide have attracted considerable interest. Among them, nitrosyl ruthenium complexes have been proposed as an attractive photodynamic therapeutic agents in biomedicine and in tumor treatment. We have designed and synthesized several ruthenium nitrosyl complexes that release NO rapidly when exposed to visible light. A series cis-{Ru-NO}⁶ nitrosyls with various dicarboxamide tetradentate ligands, namely, [(ebpp)Ru(NO)(Cl)] (1), [(4-Me)₂ebpp)Ru(NO)(Cl)] (2), [(4-OMe)₂ebpp)Ru(NO)(Cl)] (3), [(5-Bu)₂ebpp)Ru(NO)(Cl)] (4), [(3-IQ))Ru(NO)(Cl)] (5), [(1-IQ))Ru(NO)(Cl)] (6), have been successfully developed and experimentally proved to be sensitive to visible light. The quantum yields of NO photorelease at 400 nm (ϕ_{400}) increase in the order of 6 > 5 > 3 > 2, 4 > 1. We present here other evidences of photoactivated NO-releasing and other properties monitored by UV-VIS, IR, NMR, EPR, Femtosecond IR and X-ray crystallography.

Poster Presentation : **INOR.P-67**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

New Bisquinoline Cu(I) complex for Catechol Oxidase Activity

Eun su Chae, Jang Hoon Cho, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Copper enzymes are often found in many important biological processes. They are classified into several types depending on environmental characteristics. Among them, type III is a group of enzymes containing a dicopper center of which each metal ion is surrounded by three histidines. Catechol oxidase is one of the type III enzymes, catalyzing the oxidation of catechol to quinone. Many copper complexes mimicking catechol oxidase reaction have been reported. In this study, we have developed a new ligand with quinoline derivative to form a monovalent copper complex. Interestingly, the complex shows catechol oxidase activity in the presence of hydrogen peroxide. In this poster, we display the reaction pathway of catechol oxidase activity of the complex, based on the experimental evidences collected during the course of the oxidation of 3,5-di-ter-butylcatechol to 3,5-di-ter-butyl-o-quinone.

Poster Presentation : **INOR.P-68**

Inorganic Chemistry

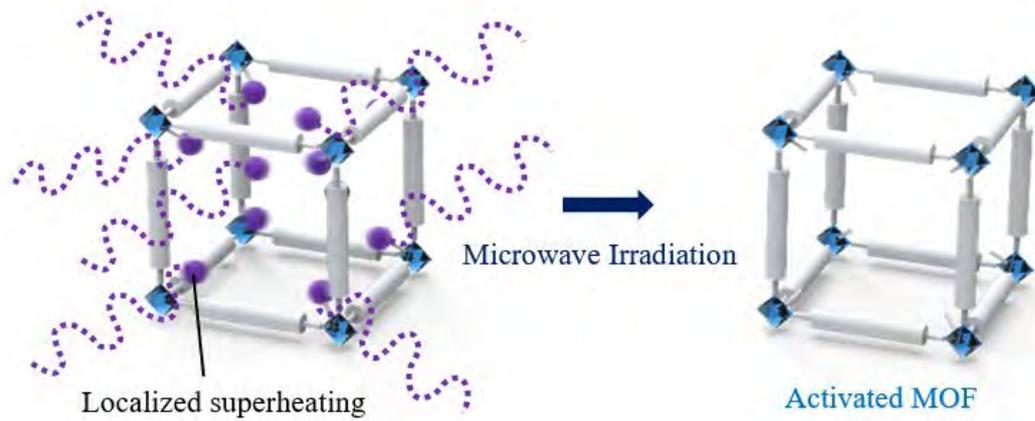
Exhibition Hall 2, THU 11:00~12:30

Practical Use of Microwave for Activation of Metal-Organic Frameworks under Ambient Condition

Eun Ji Lee, Nak Cheon Jeong*

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

Metal-organic frameworks (MOFs) are an interesting class of porous materials that are self-assembled by coordination bonding between metal node and organic ligand. Open coordination site (OCS) in MOFs, which is coordinatively unsaturated sites, has proven to play an important role in various applications of MOFs, such as molecule separation, energy storage, electronic conduction, ionic conduction, catalysis, and sensing. To utilize the OCS for such applications, activation process, which is a process to remove coordinated molecules at OCSs, is essentially required. To date, thermal activation (TA), an activation process normally conducted by applying thermal energy higher than the bond dissociation energy of solvent molecules in its extent, has been the most popularly used method. However, TA process needs to maintain high vacuum ($> 10^{-3}$ torr) for approximately 20 hours even at high temperature. Thus, this process requires extra-equipment such as schlenk line connected to a vacuum pump and electric heater in order to make the conditions. Meanwhile, microwave accelerates the rotational motion of molecules. In the aspect of thermodynamics, the excited molecule in its rotational motion is promptly relaxed, and subsequently, the relaxation energy is converted to thermal energy. We hypothesized that solvents molecules residing in the nanospace of MOF can be excited in rotational motion by absorbing microwave, and the subsequent rotational relaxation can emit nanoscale thermal energy. By utilizing this thermal energy, we further hypothesized that both coordinated solvent molecules and pore-filled solvent molecules can be removed. In this presentation, we demonstrate that applying microwave is an efficient method for the activation of OCS-containing MOFs. More precisely, we observed that MOFs such as HKUST-1 and MOF-74 series can be completely activated under ambient conditions.



Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Characterizations of 1,1-Diethyl (or Dihexyl or Diisopropyl)-2,5-bis{(trimethylsilyl)ethynyl}-3,4-diphenyl-siloles

Jong Wook Lim, Young Tae Park^{1,*}

Keimyung University, Korea

¹*Department of Chemistry, Keimyung University, Korea*

2,5-Dibromo-1,1-diethyl (or dihexyl or diisopropyl)-3,4-diphenyl-siloles were prepared by reactions of diethyl (or dihexyl or diisopropyl)-bis(phenylethynyl)silanes with lithium naphthalenide, anhydrous ZnCl₂, and *N*-bromosuccinimide (NBS), respectively. Palladium chloride, copper iodide, and triphenylsophine as co-catalyst were used to replace two bromine groups of the prepared siloles with trimethylsilylacetylene (TMSA) under the reaction condition of diisopropylamine as solvent. The crude products were refined by recrystallization or column chromatography in the solvent of hexane. The product materials were characterized by ¹H, ¹³C, and ²⁹Si NMR. We also studied the properties of materials by UV-vis absorption, excitation and fluorescence emission spectroscopic methods. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2017R1D1A3B03028014).

Poster Presentation : **INOR.P-70**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Functionalized Metal-Organic Frameworks and Mixed Matrix Membrane Composites

Jooyeon Lee, Myungeun Seo^{1,*}, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

¹*Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea*

Metal-organic frameworks (MOFs) are emerging, porous, crystalline materials for various applications such as molecular storage, molecular separation, sensor, and catalysis. However, their crystalline or powdery forms restrict precise applications in the practical point. To solve this handling issues, the composite synthesis of MOF with mixed matrix membranes (MMMs) have been intensively studied in the world. Recently, we have introduced thiol-ene photo-click chemistry for covalently cross-linked MOF-MMM synthesis. This strategy allows high MOF loading (up to 60 wt%) without particle aggregation.¹

In this presentation, further functionalization on the MOF-MMM will be discussed. The thiol-ene photo-click chemistry was successfully utilized for functionalized MOFs to fabrication with MMM. The detail synthetic preparation of MOFs and characterization data will be discussed.

Reference

1. Satheeshkumar, C.; Yu, H.-J.; Park, H.; Kim, M.*; Lee, J.-S.*; Seo, M.* *J. Mater. Chem. A*, **2018**, *6*, 21961.

Poster Presentation : **INOR.P-71**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Fine-Tuning on Pillared Metal-Organic Frameworks for Carbon Dioxide Fixation Catalysts

Dasom Kim, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs) are constructed by metal clusters (or ions) and organic ligands. Each multitopic carboxylic acids or N-donating pillar ligands are representative organic ligands for MOF synthesis. In addition, both carboxylic acid ligands and N-donating pillar ligand were employed together for pillared MOFs such as DMOF (dabco MOF) and BMOF (bpy-MOF). In this presentation, our recent study about fine-tuning of pillared MOFs for catalytic carbon dioxide fixation will be discussed.¹ Three-components (i.e., metal, carboxylic acid, and pillar ligand) were controlled to find best combination for carbon dioxide cycloaddition catalysts. The detail comparison data as well as characterization of MOFs will be discussed.

Reference

1. Noh, J.; Kim, D.; Lee, J.; Yoon, M.; Park, M.-H.; Lee, K.-M.; Kim, Y.; Kim, M. *Catalysts*, **2018**, *8*, 565.

Poster Presentation : **INOR.P-72**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Large-area Junctions of N-Heterocyclic Carbene-based Self-Assembled Monolayers, and Their Tunneling and Thermopower Properties

Seohyun Kang, Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

This presentation focuses on fabrication of large-area junctions of *N*-heterocyclic carbene (NHC)-based self-assembled monolayers (SAMs) and the length-dependence of tunneling current and thermopower in the junctions. Oligophenylene-NHC molecules of different lengths are chemisorbed on gold substrates, and the resulting monolayers are used to form large-area junctions with soft top-electrode comprising eutectic gallium-indium alloy (EGaIn) covered with a conductive native oxide layer. Our experimental results reveal that tunneling current across the junctions decreases with the increasing molecular length, showing tunneling decay coefficient and injection current density of $1.93 \pm 0.03 \text{ n}_{\text{ph}}^{-1}$ and $-0.64 \pm 0.02 \text{ A/cm}_2$ at +1.0 V, respectively. The identical junctions are used for thermoelectric measurements, and we observe that the Seebeck coefficient increases linearly with the increasing molecular length. The increase rate of Seebeck coefficient and the interfacial thermopower are $2.1 \text{ V} \pm 0.4 \mu\text{V} \cdot (\text{K} \cdot \text{n}_{\text{ph}})^{-1}$ and $8.2 \pm 0.8 \mu\text{V/K}$, respectively. Our work demonstrates for the first time the length-dependence of tunneling current density and thermopower for NHC-based large-area junctions.

Poster Presentation : **INOR.P-73**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

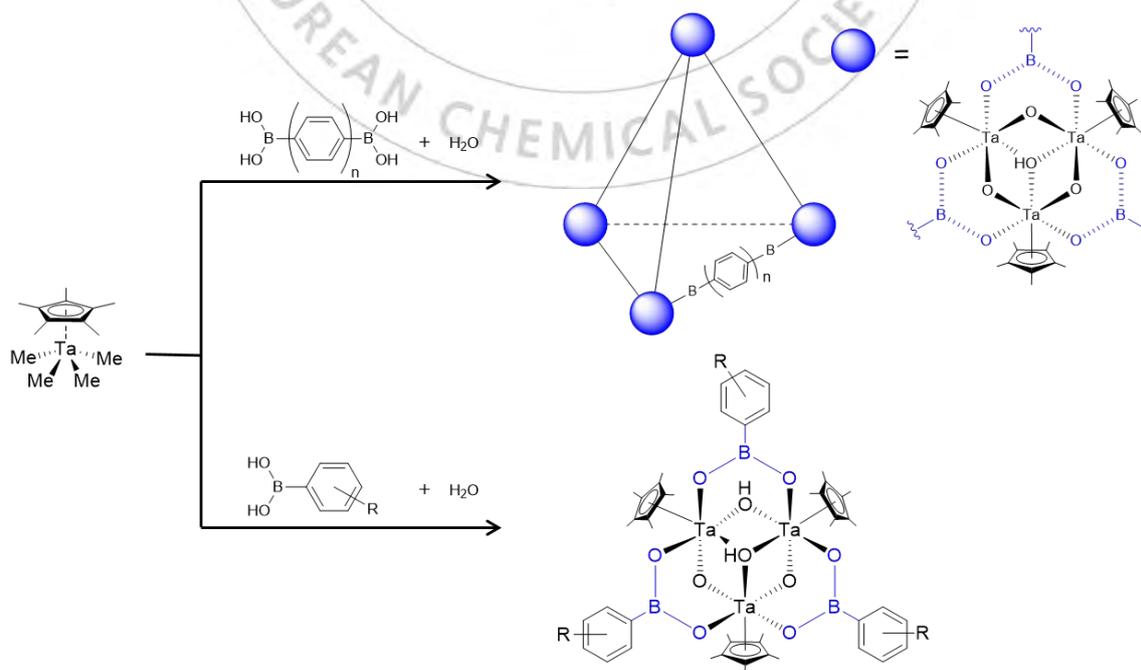
Preparation and structural studies for Ta-cluster based coordination cages

Younghun Kim, Philjae Kang¹, YeonJeong Lee, Minji Jeong, Moon-gun Choi*

Department of Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Hallym University, Korea*

Trimetallic tantalum clusters based neutral cages and cavitands is prepared by a reaction of $[\text{Cp}^*\text{Ta}(\text{Me})_4]$ ($\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$) and various boronic acids $\text{RB}(\text{OH})_2$ or $\text{R}\{\text{B}(\text{OH})_2\}_2$ via coordination self-assembly. Monotopic ligands $\text{RB}(\text{OH})_2$ lead a formation of metallocavitands and ditopic ligands $\text{R}\{\text{B}(\text{OH})_2\}_2$ lead a formation of V_4E_6 ($\text{V} = \text{vertex}$, $\text{E} = \text{edge}$) type of tetrahedral metallocages. Each products consists of $\{[\text{Cp}^*\text{Ta}]_3(\mu^2\text{-OH})(\mu^2\text{-O})_2(\mu^3\text{-OH})\}$ as a center and bridged by ligands. Especially, their cavity size is controlled by a length of ligands. Crystal structures are confirmed by a single crystal X-ray diffraction (SC-XRD) and each shows different packing structures depending on the length of ligands.



Poster Presentation : **INOR.P-74**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

New Synthetic Method in Nanocluster Using Galvanic Reaction.

Kiyoung Chang, Minseok Kim¹, Dongil Lee^{1,*}

Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Bimetallic nanoparticles have been extensively studied towards various applications due to their novel properties in the bimetal system. Among the several methods for their controlled synthesis, the galvanic reaction is particularly attractive because it enables selected the production displaying high accuracy in a single reaction step. Galvanic reaction refers to metal exchange process that occurs when two different metals are in contact, where the more noble metal is reduced by less noble metal. Metal nanoclusters composed with a few to a hundred of metal atoms and functional ligand give a special advantage for controlling the reaction producing desired bimetallic materials. In this poster, bimetallic nanocluster, MAg₂₄ (M=Pt, Pd, Au, Ni), was synthesized by using galvanic reaction, which is a metal exchange of silver nanocluster (Ag₂₅) with each more noble metal cations. Only one Pt, Pd, and Au atom were successfully replaced in Ag₂₅, whereas NiAg₂₄ was not prepared due to the lower nobility of Ni than Ag₂₅. The nobility was determined by electrochemical reduction potential. NiAg₂₄ was successfully synthesized only after the nobility of Ag₂₅ was tuned by reduction reaction towards less novel than that of Ni metal. This result implies that the galvanic reaction can be tuned by controlling metal nobility in nanocluster system. These findings help to understand the mechanism for synthesizing metal nanoclusters and lead to clear design guidelines for developing new bimetallic nanoclusters.

Poster Presentation : **INOR.P-75**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

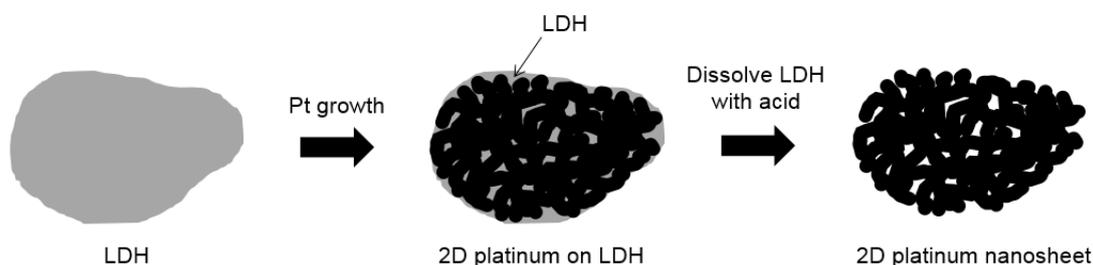
Capillaries Inspiring 2D Pt Nanosheets on Metal-Al Layered Double Hydroxide

Sunwoo Jang, Anubhab Acharya¹, In Su Lee*

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

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

Among various kinds of 2D nanomaterials, 2D metallic nanomaterials have recently received extensive research interest because of their anisotropic structure, fascinating properties, unique surface chemistry, and promising application in catalysis, sensing, photothermal therapy, solar cells and so on. Here, we have grown 2D platinum with MgAl-LDH(Layered double hydroxide) as a template. This synthetic method is based on a seeding and fast autocatalytic growth approach in which an aqueous solution of platinum salt is reduced by ascorbic acid. It is well known that the collaboration of materials including platinum and transition metal has high efficiency as an electrocatalyst. So we extended our research to LDH with transition metal in the same way. The 2D-Pt-LDH electrocatalysts were expected to have dramatically enhanced its catalytic activity.



Poster Presentation : **INOR.P-76**

Inorganic Chemistry

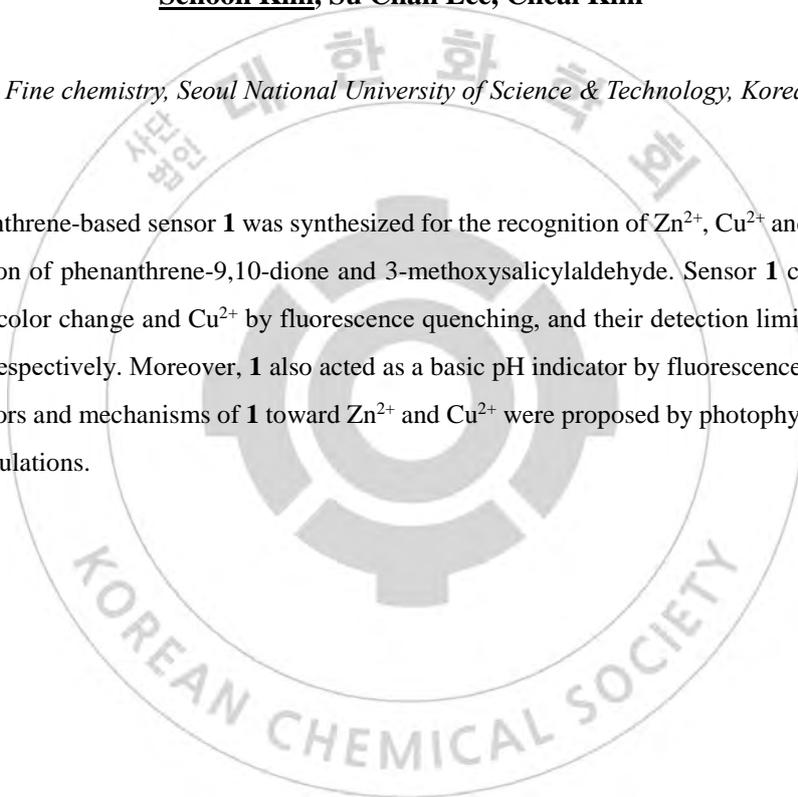
Exhibition Hall 2, THU 11:00~12:30

Fluorescent detection of Zn²⁺ and Cu²⁺ by a phenanthrene-based multifunctional chemosensor that acts as a basic pH indicator

Sehoon Kim, Su Chan Lee, Cheal Kim*

Fine chemistry, Seoul National University of Science & Technology, Korea

A novel phenanthrene-based sensor **1** was synthesized for the recognition of Zn²⁺, Cu²⁺ and basic pH range by an integration of phenanthrene-9,10-dione and 3-methoxysalicylaldehyde. Sensor **1** could detect Zn²⁺ by fluorescent color change and Cu²⁺ by fluorescence quenching, and their detection limits were 0.43 μM and 0.18 μM, respectively. Moreover, **1** also acted as a basic pH indicator by fluorescence quenching. The sensing behaviors and mechanisms of **1** toward Zn²⁺ and Cu²⁺ were proposed by photophysical studies and theoretical calculations.



Poster Presentation : **INOR.P-77**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

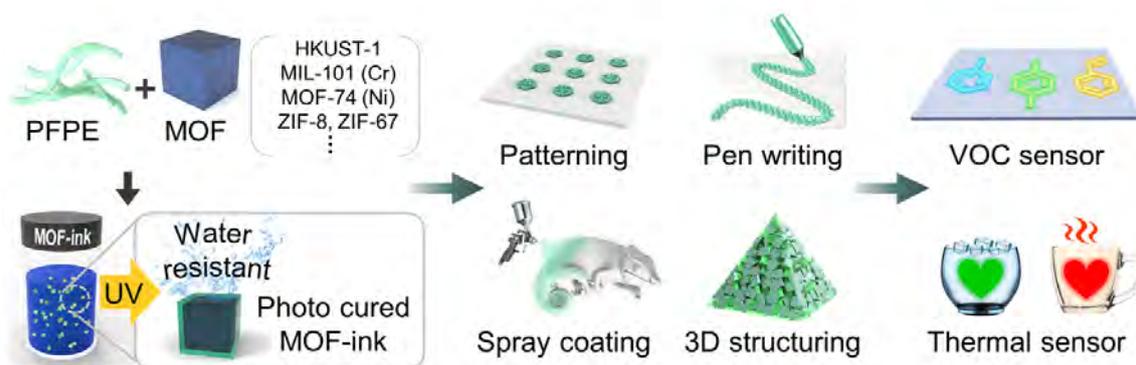
Versatile Processing of Metal-Organic Framework-Fluoropolymer Composite Inks with Chemical Resistance and Sensor Applications

Jin Yeong Kim, Hoi Ri Moon*, Dong Pyo Kim^{1,*}

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

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

We report a new class of MOF inks with a water-repellent, photocurable fluoropolymer (PFPE) having up to 90 wt% MOF loading. These MOF inks enable to process various MOFs through spray coating, pen writing, stencil printing, and molding at room temperature. Upon UV-curing, the hydrophobic PFPE matrix efficiently blocks water permeation but allows accessibility of chemicals into MOF pores, thereby freeing the MOF to perform its unique function. Moreover, by introducing functional MOFs we successfully demonstrated a water-tolerant chemosensor for a class of aromatic pollutants in water and a chemical-resistant thermosensor for visualizing temperature image. This approach would open up innumerable opportunities for those MOFs that are otherwise dormant.



Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Fluorescent detection of Zn(II) and In(III) and colorimetric detection of Cu(II) and Co(II) by a versatile chemosensor

Haeri So, Sojeong Lee, Cheal Kim*

Fine chemistry, Seoul National University of Science & Technology, Korea

A new versatile chemosensor **1** ((Z)-N'-(quinolin-2-ylmethylene)furan-2-carbohydrazide), based on quinoline and furan, has been synthesized. Sensor **1** showed immediate responses toward Zn²⁺ and In³⁺ ions through selective fluorescence enhancement in different solvent conditions, respectively. In addition, sensor **1** could detect Cu²⁺ and Co²⁺ by “naked eye” color changes from colorless to pale yellow in a near-perfect aqueous solution. This observation was the first case that a single sensor can detect the four metal ions. The binding modes of **1** to Zn²⁺, In³⁺, Cu²⁺ and Co²⁺ were verified through Job plots and ESI-mass spectrometry analyses. The limits of detection (0.33 μM, 0.23 μM and 0.06 μM) for Zn²⁺, Cu²⁺ and Co²⁺ were far lower than the World Health Organization (WHO) guidelines (76 μM for Zn²⁺ and 31.5 μM for Cu²⁺) and Department of Environmental Protection (DEP) guideline (1.7 μM for Co²⁺) for drinking water. Moreover, sensor **1** could quantify Zn²⁺ and Co²⁺ in water samples. The sensing mechanisms of Zn²⁺, In³⁺ and Cu²⁺ by sensor **1** were explained by theoretical calculations.

Poster Presentation : **INOR.P-79**

Inorganic Chemistry

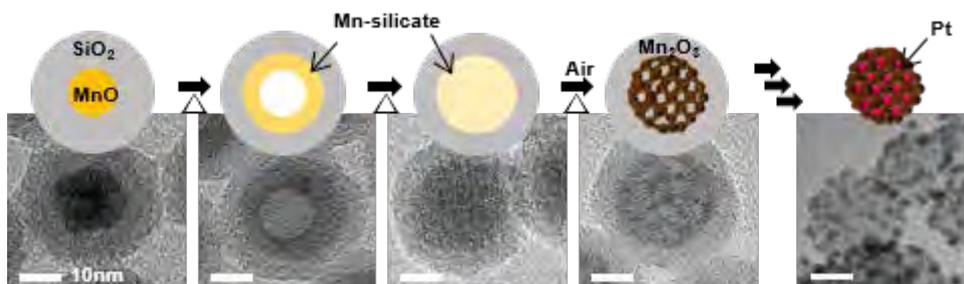
Exhibition Hall 2, THU 11:00~12:30

Conversion Chemistry of Manganese Silicate in Nanospace: Solid-state Synthetic Route towards Porous Metal Oxide

Taewan Kwon, Kyun Sang Ji, Jeonghun Choi, In Su Lee*

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

By utilizing the nanospace-confinement strategy with silica nanosphere as reaction medium, the unexpected transformation behavior of the nanosized manganese silicate could be observed in high temperature environment. The investigation of MnO nanocrystal (NC) within a silica nanosphere with increasing the annealing temperature showed the stepwise transformation from solid to hollow and back to solid interior structures. This conversion could be elucidated by the multistep process, including the formation of hollow Mn-silicate layer with lowered glass transition temperature (T_g) and its subsequent void-filling diffusion, which are attributed to the space-confinement effect within a nanoscale environment. In addition, the thermal oxidation of the resultant low-density Mn-silicate phase led to an important distinctive phase-segregation phenomenon, credited to the nanoscopic reaction medium circumscribed by a tight silica shell, which creates a highly porous nanostructure of the phase-segregated manganese(III) oxide (p-Mn₂O₃). The p-Mn₂O₃, isolated from a silica medium without affecting the overall morphology and porosity, was employed as catalyst-support which inhibits the problematic thermal sintering process for tiny Pt NCs (~3 nm) even at high temperature of 400 °C. The p-Mn₂O₃-supported Pt NCs have demonstrated a superior long-term stability in catalyzing oxygen reduction reaction to those of commercial Mn oxide based analogue and Pt/C catalyst.



Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

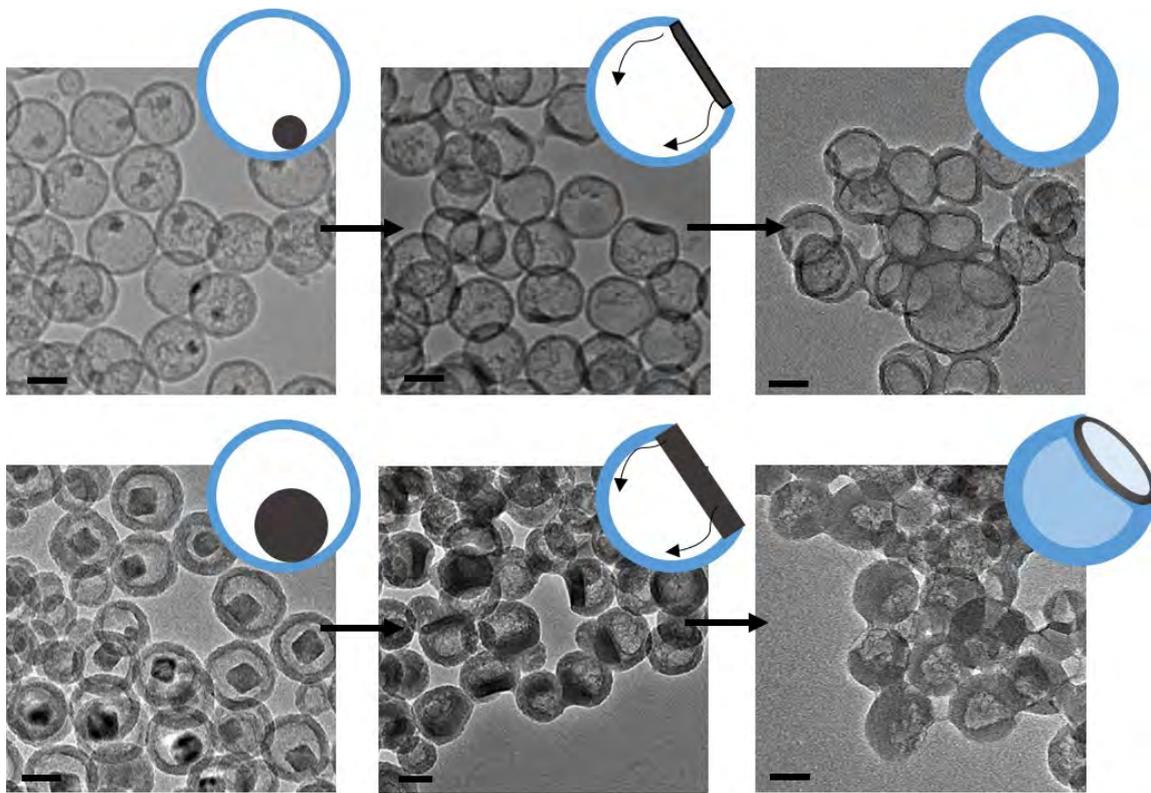
Thermal transformation of MnO@h-SiO₂ by solid-state reaction

Seonock Kim, SeonYeong Choi¹, In Su Lee*

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

¹Advanced Materials Science, Pohang University of Science and Technology, Korea

We already have observed the transformation of the nanosized Mn-silicate phase in nanospace-confined environment using silica nanosphere. By using yolk-shell structure of MnO@h-SiO₂, we investigated the structural transformation with increasing the annealing temperature, time and Mn contents. The investigation showed the stepwise transformation from asymmetric Mn-silicate@h-SiO₂ nanoparticle like janus structure to squashed hollow silica nanoparticle at low Mn content and the bowl-shaped particles were obtained as the final structure at high Mn content. This conversion process could be elucidated by the formation of localized Mn-silicate region with lowered glass transition temperature (T_g) and its subsequent diffusion. Through this observation, we can easily convert the structure of particle and synthesize hybrid structure with functionalized material by simple solid-state reaction.



Scale bar : 50nm



Poster Presentation : **INOR.P-81**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Heterometal coordinated concanavalin A and its trimeric complexation

Seung Jae Lee^{*}, Ha Ra Jang¹, Yung Min Lee¹

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

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

Concanavalin A (ConA) interacts with carbohydrates as a lectin, and recent reports proposed its application for detecting a diversity of viruses and pathogens. Structural studies have detailed the interaction between ConA and carbohydrates and the metal coordination environment with manganese and calcium ions (Mn-Ca-ConA). In this study, ConA was crystallized with a cadmium-containing precipitant, and the refined structure indicates that Mn was replaced by Cd (Cd-Ca-ConA). The structural comparison with ConA demonstrates that the metal-coordinated residues of Cd-Ca-ConA, that is Glu8, Asp10, Asn14, Asp19, and His24, do not have conformational shifts, but residues for sugar binding, including Arg228, Tyr100, and Leu99, reorient their side chains, slightly. Previous studies demonstrated that excess cadmium ions can coordinate with other residues, including Glu87 and Glu183, which were not coordinated with Cd in this study. The trimeric ConA in this study coordinated Cd with other residues, including Asp80 and Asp82, for complex generation. The monomer does not have specific interaction near interface regions with the other monomer, but secondary cadmium coordinated with two aspartates (Asp80 and Asp82) from monomer 1 and one aspartate (Asp16) from monomer 2. This study demonstrated that complex generation was induced via coordination with secondary Cd and showed the application potential regarding the design of complex formation for specific interactions with target saccharides.

Poster Presentation : **INOR.P-82**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Oxidation of methane through component interactions from type II methanotrophs

Seung Jae Lee*, **Heeseon Yoo¹**, **Chungwoon Yoon¹**, **Jaewoong Park¹**

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

¹*Department of chemistry, Chonbuk National University, Korea*

Methane hydroxylation through methane monooxygenases (MMOs) is a key aspect due to their control of the carbon cycle in the ecology system and recent applications of methane gas in the field of bioenergy and bioremediation. Methanotropic bacteria perform a specific microbial conversion from methane, one of the most stable carbon compounds, to methanol through elaborate mechanisms. MMOs express particulate methane monooxygenase (pMMO) in most strains and soluble methane monooxygenase (sMMO) under copper-limited conditions. The mechanisms of MMO have been widely studied from sMMO included in the bacterial multicomponent monooxygenase (BMM) superfamily. Mechanism studies of sMMO have been intensively studied by the supports of advanced biophysics, especially in the *Methylococcus capsulatus* (Bath) and *Methylosinus trichosporium* OB3b strains. Structural studies of three components of sMMO, a hydroxylase (MMOH), a regulatory component (MMOB), and a reductase (MMOR), have provided crucial information about their catalytic activities. In this study, we report successful growing and expression from type II methanotrophs, *Methylosinus sporium* 5.

Poster Presentation : **INOR.P-83**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of New Copper Precursors for Atomic Layer Deposition of Cu Oxide Thin Films

Sunyoung Shin, Bo Keun Park, Taek-Mo Chung^{1,*}

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea

¹*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Copper oxide is gaining attention due to favorable interesting characteristics such as environmentally friendly, being cost effective, and having reconfigurable electronic structures. Among many copper oxides, cuprous oxide (Cu_2O) and cupric oxide (CuO) are used in various applications due to their excellent electrical properties. For instance, Cu_2O and CuO show the *p*-type characteristic when they have cubic and monoclinic crystal structures. Such characteristic can be used as gas sensor, anode materials in batteries, thin film transistors (TFTs), solar cells, and photo-catalysts. Generally, chemical vapor deposition (CVD) and atomic layer deposition (ALD) are required to form uniform surface on the substrate. CuO_2 or CuO can be selectively deposited by controlling the oxidation state of the Cu(II) precursors and/or reactant gas. In this study, we synthesized novel Cu(II) complexes as next generation precursors for ALD deposition technique. Synthesized complexes were fully analyzed by various analysis equipments such as infrared spectroscopy (IR), elemental analyses (EA), thermogravimetric analysis (TGA), and single crystal X-ray diffraction.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Boost-up Electrochemical Performance of MOFs via Confined Synthesis within Nanoporous Carbon Matrices for Supercapacitor and Oxygen Reduction Reaction Applications

Hee Soo Kim, Min seok Kang, Jeho Suh, Won Cheol Yoo^{1,*}

Department of Applied Chemistry, Hanyang University, Korea

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

Utilizations of metal-organic frameworks (MOFs) for electrochemical applications are significantly limited by insulating nature and mechanical/chemical instability thereof. One promising approach for the deployment of conventional MOFs in electrochemical applications is to fabricate MOF-based hybrids (MBHs) with conductive materials, which facilitate effective electron transfer via conductive additives between MOFs. Herein, we present a facile method for effective filling of Cu- and Ni-HKUST-1 (Hong Kong University of Science and Technology, and denoted hereafter Cu-/Ni-MOF) inside 3D ordered mesoporous carbon (24 nm, mC), 3D ordered N-doped macroporous carbon (300 nm, NMC), and 3D ordered macroporous carbon (300 nm, MC), denoted as MOF@mC, MOF@NMC, and MOF@MC, respectively. The MOF@carbon matrix (MOF@CM) composites were intended for use as electrodes for electric double layer capacitors (EDLCs) and as electrocatalysts for the oxygen reduction reaction (ORR). EDLC performance of MOFs can be significantly improved by facilitating electron transfer through 3D conductive CM, reducing the electron pathway within insulating MOF using CM with small pores, and choice of metal center with pronounced faradaic nature. Ni-MOF@mC exhibited superior specific surface area normalized areal capacitance ($26.5 \mu\text{F}/\text{cm}^2$), exceeding most carbons and MOF-based EDLCs and outstanding long-term stability (91% @ 5000th). Furthermore, Cu-MOF@mC resulted in pronounced ORR activities, excellent methanol tolerance, and long-term stability. It is clearly demonstrated that conventional MOFs can be utilized for EDLC and ORR when conjugated with a 3D-connected nano-sized CM.

Poster Presentation : **INOR.P-85**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Model Complex of [NiFe]-Carbon Monoxide Dehydrogenase Active Site using Aromatic Spacer

Seungjin Song, Junhyeok Seo*

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

Carbon monoxide dehydrogenase (CODH) is a family of enzymes, that promotes the conversion of CO to CO₂. The enzymes are categorized as [NiFe]- and [MoCu]-CODH according to the metal ions in the active sites. The [NiFe]-CODH, functioning under anaerobic conditions, is known to be also active for the reversible CO₂ reduction. According to the X-ray crystal structure, the enzyme active site contains a Ni(II) ion in the square planar geometry and a high-spin Fe(II) in the tetrahedral coordination. In particular, as seen in another X-ray crystal structure of the 'Ni-C(O)O-Fe' moiety, the FeS cluster maintains the Ni and Fe centers by 2.87 Å. The interstitial distance seems essential for the interaction of the CO₂ molecule with the 'frustrated' Lewis pair of the Ni and Fe centers. Since the time that the crystal structure of the enzyme active site is known, many structural analogues have been synthesized by others; however, so far known models never showed the enzyme-like reactivity with CO₂ or CO. We synthesize model complexes of the [NiFe]-CODH active site to understand the structural meaning of the active site, and furthermore develop the small molecular catalysts for the CO₂ reduction. Currently, we model the Ni active center by a Ni-pincer complex, and then conjugate a high spin Fe(II) complex using aromatic spacers. The molecular framework would likely position the Ni/Fe active centers closely to capture CO₂, and the synthesized model complexes are tested for the reduction of CO₂.

Poster Presentation : **INOR.P-86**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A multifunctional selective “turn-on” fluorescent chemosensor for detection of Group IIIA ions Al^{3+} , Ga^{3+} and In^{3+}

Pyeong An Kim, Yuna Seo, Cheal Kim*

Fine chemistry, Seoul National University of Science & Technology, Korea

A versatile chemosensor **1** (E)-2-(((8-hydroxy-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-9-yl)methylene)amino)-1H-benzo[de]isoquinoline-1,3(2H)-dione, based on naphthalimide and julolidine moieties, was developed for a highly distinguishable and selective recognition of group IIIA metal ions (Al^{3+} , Ga^{3+} and In^{3+}). Sensor **1** exhibited significant ‘off-on’ fluorescence responses at 488 nm in the presence of Al^{3+} and at 570 nm in the presence of Ga^{3+} and In^{3+} . The same emission of Ga^{3+} and In^{3+} could be distinguished through different color changes (from colorless to yellow for Ga^{3+} and no color change for In^{3+}). Binding constants of **1** for Ga^{3+} and In^{3+} are the highest ones among those previously known for the organic chemosensors, to date. The 2:1 binding structures between **1** and Al^{3+} , Ga^{3+} and In^{3+} were proposed by ESI-mass and Job plot, and theoretical calculations.

Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A dual target chemosensor for the fluorometric detection of In^{3+} and colorimetric detection of Fe^{3+}

Duo Zhang, Chang Joo Rha, Cheal Kim*

Fine chemistry, Seoul National University of Science & Technology, China

A new dual target chemosensor **1**, 1,1'-((1E,1'E)-((thiobis(ethane-2,1-diyl))bis(azanylylidene))bis(methanylylidene))bis(naphthalen-2-ol), was prepared by the reaction of a hydroxy-naphthaldehyde and a thiobis(ethylamine). Sensor **1** detected In^{3+} with turn-on fluorescence and Fe^{3+} via the change of color from colorless to pale violet. The sensing behaviors of **1** toward In^{3+} and Fe^{3+} were studied through photophysical experiments, ESI-mass, NMR titration, and theoretical calculations. In particular, **1** can discriminate In^{3+} from Al^{3+} and Fe^{3+} from Fe^{2+} . Limits of detection for the analysis of In^{3+} and Fe^{3+} ions turned out to be $5.89 \mu\text{M}$ and $0.30 \mu\text{M}$, respectively. In addition, sensor **1** functioned practically as a naked-eye test strip for Fe^{3+} and could be recycled by using EDTA for In^{3+} and DFO for Fe^{3+} .

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

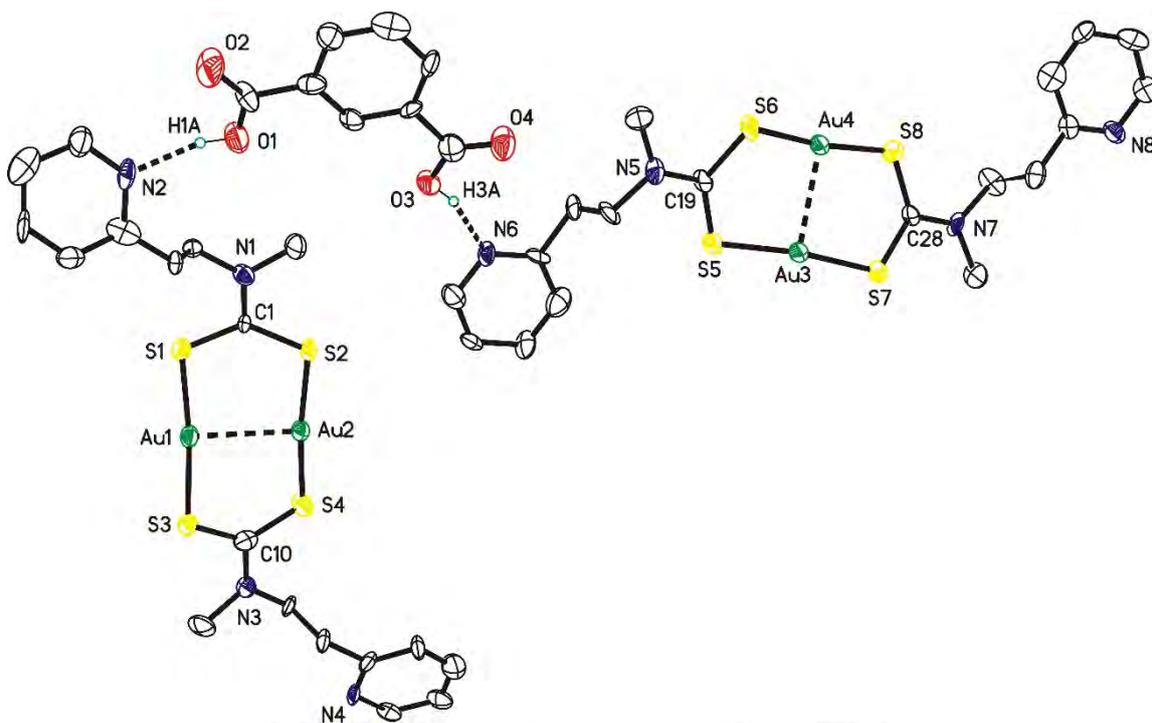
Exhibition Hall 2, THU 11:00~12:30

Adduct effects on structure and luminescence in a series of new dithiocarbamatogold(I) complexes

HeeHun Moon, Sung Kwang Lee, Young-A Lee*

Department of Chemistry, Chonbuk National University, Korea

Reaction of $[\text{AuCl}(\text{SMe}_2)]$ with $\text{NaL}\cdot\text{H}_2\text{O}$ (L = ethyl(pyridine-4-yl methyl)dithiocarbamate (epdtc) or methyl(2-(pyridin-2-yl)ethyl)dithiocarbamate (mpdtc)) affords a series of neutral dinuclear gold(I) complexes bridged by each dithiocarbamate ligand, $[\text{Au}(\text{L})]_2$. The successive reaction of $[\text{Au}(\text{L})]_2$ with organic acids such as isophthalic acid (m-pa) and maleic acid (ma) produces 1:1 adducts, $[\text{Au}(\text{L})]_2\cdot(\text{organic acid})$. The crystal structure of $[\text{Au}(\text{L})]_2\cdot(\text{m-pa})$ is a 1D polymer formed via hydrogen bonds between the free pyridyl and the carboxylic acid moiety. For the dinuclear moiety, strong intradinuclear aurophilic interactions ($\text{Au}(\text{I})\text{--Au}(\text{I}) = 2.7783(8) \text{ \AA}$ and $2.7525(7) \text{ \AA}$) exist, but interdinuclear interactions are weak ($3.2551(8)\text{--}3.2733(8) \text{ \AA}$). The dinuclear gold(I) complexes, $[\text{Au}(\text{epdtc})]_2$ and $[\text{Au}(\text{mpdtc})]_2$, show a bright luminescence at 562.5 and 552.0 nm in solid state, respectively, but their organic acid adducts, $[\text{Au}(\text{L})]_2\cdot(\text{organic acid})$, have no luminescent properties. This dramatic difference in properties between the gold(I) complexes and their adducts may be ascribed to the weakness of the internuclear $\text{Au}(\text{I})\text{--Au}(\text{I})$ interaction including crystal packing.



Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

**Synthesis and structural analysis of Sr complex of tridentate ligands :
[Sr(L)²(btsa)²] (L = (bdmpH), (bdmampH) and (dadambH)) (btsa =
bis(trimethylsilyl)amine)**

Chanwoo Park, Taek-Mo Chung^{1,*}, Bo Keun Park², Chang Seop Hong³

Chemistry, Korea University, Korea

¹*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

²*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

³*Department of Chemistry, Korea University, Korea*

The heavier alkaline-earth metals with high sublimation temperature such as calcium, strontium, and barium are key components of superconductors and colossal magnetoresistive thin film. [1-2] Among the various ways to deposit thin films, metal-organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) have possibility such as large-area growth, delicate composition control and high film uniformity. Because the application of alkali metals to these depositions requires highly volatile properties, our group's study has focused on design strontium complex with volatile and stability at high temperature. [3] Strontium complexes were synthesized by reacting Sr(btsa)²(DME)² with tridentate ligands. (bdmpH, bdmampH and dadmbH. Synthesized strontium complexes were fully characterized by single crystal XRD analysis, H - NMR, elemental analysis, and thermal stability was analyzed by TGA. All complexes existed in a trigonal bipyramid, where strontium metals have five coordination bonds of nitrogen and oxygens from the tridentate type ligands. References [1] D. L. Schulz, T. J. Marks, Adv. Mater. 1994, 6, 719. [2] N. Zurauskiene, S. Balevicius, V. Stankevici, J. Parseliunas, S. Kersulis, A. Abrutis, V. Plausinaitiene, Acta Phys. Pol. A 2009, 115, 1136. [3] S. M. George, B. K. Park, C. G. Kim,* and T. M. Chung, Eur. J Inorg. Chem. 2014, 2002–2010.

Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Aligned Microporous Organic Network Tubes for the AIE-Based Sensing of Explosives

Sanghyun Ryu, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Aligned Microporous Organic Network Tubes for the AIE-Based Sensing of Explosives Sang Hyun Ryu, Seung Uk Son* Department of Chemistry, Sungkyunkwan University This presentation shows the sensing performance of conjugated microporous polymer (CMP) tubes. Using anodic aluminum oxide (AAO) plates as template, the aligned CMP tubes were engineered through the Sonogashira coupling of tetra(4-ethynyl)phenylethylene with 1,4-diiodobenzene. The length of CMP tubes was controlled in the range of 1 ~ 5 μm . In addition, the wall thickness of CMP tubes was controlled in the range of 40 ~ 60 nm by changing the amount of building blocks. The CMP-AT films showed aggregation-induced emission (AIE) because they contain tetraphenylethylene moieties. The emissions of CMP-AT films were quenched by the model explosives, nitrotoluenes, was studied. The CMP-AT-5 having longest CMP tubes with thinnest wall thickness showed the best sensing performance towards 2,4-dinitrotoluene (DNT).

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Macroporous Engineering of Conjugated Microporous Organic Network Films Bearing Tetraphenylethylenes for the Enhanced Sensing of Nitrotoluenes

Chang Wan Kang, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

This presentation shows the macroporous engineering of microporous organic network (MON) materials for enhanced sensing of nitrotoluenes. MON materials have been prepared by the transition metal catalyzed cross-coupling of organic building blocks. Although the unique microporosity of MONs enables the diffusion of guest molecules into inner MONs, the guest molecules can hinder the diffusion pathways each other, which can limit the interaction of substrates with inner functional moieties of MONs. The introduction of secondary macroporosity to the MON materials can further facilitate the diffusion of substrates. Thus, it is noteworthy that binary porosity materials have been synthesized to enhance the functionalities of organic/inorganic microporous materials. The efficient sensing of dangerous compounds has been an important research subject. Recently, the phenomenon of aggregation-induced emission (AIE) has been utilized as a new principle in emission-based sensing materials. For example, MONs bearing tetraphenylethylene (TPE) moieties showed emission through the aggregation-induced suppression of intramolecular motions and were applied for the sensing of harmful compounds. Moreover, the film form of emissive MON materials can be engineered to facilitate the sensing processes. We have demonstrated that the performance of MON materials is critically dependent on the morphological structures of MON materials. In this regard, macroporous MON-Fs (MA-MON-Fs) were engineered using assembled silica spheres as templates. The MACMP-Fs showed much better sensing performance toward nitrotoluenes with Stern–Volmer constants (K_{sv}) of up to $1.39 \times 10^5 \text{ M}^{-1}$, compared with CMP-Fs (K_{sv} up to $5.57 \times 10^4 \text{ M}^{-1}$). The sensing performance of the MA-MON-F is superior to those of recent emissive MON materials, which is attributable to the additional macroporosity of the MON-F

Poster Presentation : **INOR.P-92**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Hollow microporous organocatalysts bearing pyrrolidines

Kyoungil Cho, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Hollow microporous organic polymers were synthesized by the Sonogashira coupling of tetrakis(4-ethynylphenyl)adamantane with 1,4-bis(trimethylsilylethynyl)-2,5-dibromobenzene on 300nm silica template. Silica template and trimethylsilylacetylene group were removed by the treatment of hydrofluoric acid. Through post synthetic modification, microporous organocatalysts bearing pyrrolidines (H-MOP-P) were prepared. The BOC protecting groups on pyrrolidines were removed by the treatment of trifluoroacetic acid. The H-MOP-P exhibited high surface area (378 m²/g, V_{mic}: 0.14 cm³/g) and microporosity (pore sizes < 2nm). The chemical structure of H-MOP-P was characterized by infrared (IR) absorption and solid state ¹³C nuclear magnetic resonance (NMR) spectroscopy. The H-MOP-P showed high catalytic performance of asymmetric malonate additions to cinnamaldehydes.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Polymer-assisted synthesis of hierarchical mesoporous metal organic framework-A host for catalytic nanoparticles and large biomolecules

Soumen Dutta, In Su Lee*

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

We constructed highly oriented mesopores within metal-organic framework (MOF) by tuning the metal-ligand binding in presence of polyvinylpyrrolidone (PVP). Usual growth of three-dimensional-ordered zeolitic imidazolate framework (ZIF-67) is hampered through strong Co-O interaction by PVP in solution and finally it results in 30-50 nm sized large pores inside the ZIF moiety. Our methodology relies on the competitive metal-ligand interaction using common polymer which enabled the growth of mesoporous MOFs in presence of same polymer coated catalytic particles to fabricate nanoparticles encapsulated porous ZIF. By sequential addition of dissimilar nanoparticles, we are able to prepare core-shell type distributed nanoparticles inside hierarchical mesoporous ZIF. Additionally, the improved mass diffusion properties of such hierarchical frame can be utilized to capture large molecules like enzymes for desired catalytic reactions as compared to conventional solid ZIF-67.

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A highly selective fluorescent chemosensor for detecting indium(III) with a low detection limit and its application

Hangyul Lee, Soyoung Park, Cheal Kim*

Fine Chemistry, Seoul National University of Science & Technology, Korea

A highly selective chemosensor **BHC** ((E)-N-benzhydryl-2-((2-hydroxynaphthalen-1-yl)methylene)hydrazine-1-carbothioamide) for detecting indium(III) was synthesized. Sensor **BHC** can detect In(III) by a fluorescence turn-on method. The detection limit was analyzed to be 0.89 μM . Importantly, this value is the lowest among those previously known for fluorescent turn-on In(III) chemosensors. Based on the analytical methods like ESI-mass, Job plot, and theoretical calculations, the detection mechanism for In(III) was illustrated to be chelation-enhanced fluorescence (CHEF) effect. Additionally, sensor **BHC** was successfully applied to test strips.

Poster Presentation : **INOR.P-95**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Electrochemical activity of Pd@PdS core shell in ethanol oxidation reaction

Hyung Bo Shim, Heon Chul Kim, Jong Wook Hong*

Chemistry, University of Ulsan, Korea

In many industrial chemical reactions, Pd-based catalysts have excellent catalytic efficiency for fuel oxidation reaction. Pd nanoparticles also have been explored as potential hydrogen storage media. Catalyst performance for electrochemical activity can be increased by adjusting size, shape and composition. Transition metal sulfides have been found to be very important for various applications due to their special physical and chemical properties. For example, Ni-Mo-S and RuS₂ have been used for hydrodesulfurization reactions and nitrogen denitrification reactions. Pd sulfide NPs has been found to be a more promising catalyst than the other transition metal sulfides for thiophene hydrogenation and reductive N-alkylation of aromatic amines. And it has attracted attention in recent years because of the ease of formation of active sites. We synthesized carbon supported Pd@PdS core shell nanoparticles. In particular, we controlled the thickness of the sulfur. The synthesized nanoparticles were characterized by various methods such as transmission electron microscopy (TEM) and energy dispersive x-ray spectroscopy (EDS). We also confirmed their differences of the electrochemical catalytic activity in the basic electrolyte according to thickness of the sulfur.

Poster Presentation : **INOR.P-96**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Pd Nanocubes@PANI/C as Catalysts for Proton Exchange Membrane Fuel Cell

Heon Chul Kim, Hyung Bo Shim, Jong Wook Hong*

Chemistry, University of Ulsan, Korea

Proton exchange membrane fuel cell has high efficiency, low electrode reaction temperature compared other cells and it is also eco-friendly. Palladium is one of metal that can be used as catalysts for electrochemical because it has significant properties in ethanol oxidation reaction (EOR) of anode fuel oxidation reaction in PEMFCs. Controlling catalyst shape and composition at nanoscale enhances electrochemical activity of palladium catalysts. The electrochemical activity can be increased by synthesis with nano-size material. Here in, we have synthesized palladium nanocubes about ~20 nm and coated them with polyaniline (PANI). Thickness of PANI shells can be controlled. We used scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to confirm the nanoparticles were uniformly produced. Electrocatalysis properties of Pd@PANI NPs in ethanol oxidation reaction were measured by cyclic voltammetry (CV) and compared the electrochemical activity of the catalyst as a function of thickness.

Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Solution-phase growth of Cu₂O nanocubes on dispersible MoS₂ nanosheets for photocatalytic property

Eun Jin Yu, Yeji Han, Jong Wook Hong*

Chemistry, University of Ulsan, Korea

The controlled synthesis of nanohybrids composed of noble metals (Au, Ag, Pt, and Pd) and metal oxides (ZnO, TiO₂, Cu₂O and CeO₂) have received considerable attention for applications in photocatalysis, solar cells, drug delivery, surface enhanced Raman spectroscopy and various important areas. Among various metal oxides, cuprous oxide (Cu₂O), an important p-type semiconducting material with a unique optical and electrical property, is an appealing candidate for solar energy conversion, sensors, photo-catalytic degradation and coherent propagation of excitons. In addition, it has an attractive property to absorb visible light region. Two-dimensional semiconductors such as molybdenum disulfide (MoS₂) are emerging material family with wide-ranging potential applications in electronics, optoelectronics and energy harvesting. MoS₂ is one of the promising materials that can be used in nanotechnology and it can be made as a few atomic layers. The MoS₂ nanosheets composed of a few atomic layers have high surface areas, which improves the photocatalytic and photovoltaic efficiency in visible light region. In this paper, a Cu₂O/MoS₂ nanocomposite was prepared by growing Cu₂O onto MoS₂ nanosheets for photodegradation. The samples were characterized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy and UV-Vis spectrophotometry. The size of Cu₂O nanoparticles grown on the MoS₂ nanosheets is about 28-33 nm. The Cu₂O/MoS₂ nanocomposites showed greatly enhanced photocatalytic efficiency compared to the pure Cu₂O nanoparticles and MoS₂ for photodegradation of theophylline and methyl orange (MO) under visible light. The photocatalytic performances were mainly ascribed to enhanced efficiency for solar energy absorption as well as the efficient charge transportation and separation from Cu₂O to MoS₂ nanosheets.

Poster Presentation : **INOR.P-98**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Pd-based nanocubes as electrochemical catalyst for CO₂ reduction reaction

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University of Ulsan, Korea

¹*Chemistry, University of Ulsan, Korea*

Until now, the main source of energy is fossil fuels. However, the reserves of fossil fuels are being decreased and fossil fuels generates the carbon dioxide that affects the climate. Therefore, many people are developing alternative energy sources such as electric energy, hydrogen energy and natural energy. However, there are some problems. It is hard to store electricity and hydrogen energy. Natural energies are influenced by the weather. The above problems can be solved by using abundant carbon dioxide in the air. The carbon dioxide reduction reaction can produce energy sources such as methane, methanol and carbon monoxide. Currently, many metals are being studied as catalyst for CO₂ reduction reaction. Palladium is one of them. In a recent paper, it has been found that Pd hydride nanoparticles reduce the binding energy of intermediates and show high current density and faradaic efficiency in CO₂ reduction reaction. In this study, we compared Pd nanocubes and Pd based nanocubes with hydrogen, boron and phosphorus for CO₂ reduction reaction, respectively.

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

***N*-Heterocyclic Carbene Derived 3-Azabutadiene as π -Basic Component in Frustrated Lewis Pair Chemistry**

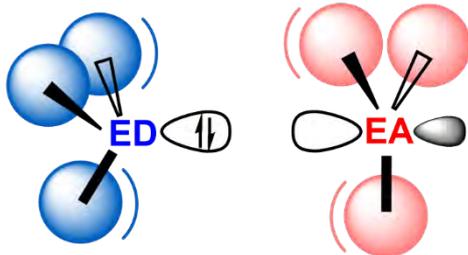
Youngsuk Kim, Liu Leo Liu¹, Douglas W. Stephan^{1,*}

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

¹*Department of Chemistry, University of Toronto, Canada*

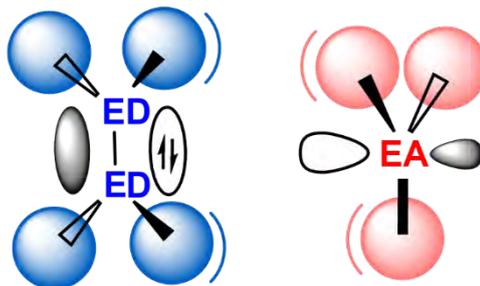
Since the seminal report of metal-free reversible hydrogen activation by p -(Mes₂P)₂C₆F₄(B(C₆F₅)₂) (Mes = mesityl) in 2006, frustrated Lewis pair (FLP) chemistry has gained tremendous success in the area of small molecule activation and has expanded dramatically to catalysis and material sciences.^[1] Lewis bases in FLP systems featuring a sterically encumbered nucleophilic center with a localized lone pair of electrons have been extensively explored (Figure 1a). However, Lewis bases featuring a delocalized π -type electron pair have been seldom encountered in FLP chemistry (Figure 1b). In the present work, we report the synthesis of NHC-derived 3-azabutadienes via a [1+1] addition reaction of NHCs with cyclohexyl isocyanide CyNC followed by a spontaneous tautomerization. The delocalized π -basicity of 3-azabutadienes in classic Lewis pair and FLP chemistry is considered, the latter of which shows facile cleavage of chemical bonds, when combined with the Lewis acidic component. Computational study including intrinsic bond orbital (IBO) analysis showcases the role of π -electrons of 3-azabutadienes in the bond activation step. Figure 1. (a) FLP system with localized donor. (b) FLP system with delocalized donor. Reference [1] G. C. Welch, R. R. S. Juan, J. D. Masuda, D. W. Stephan, *Science* 2006, 314, 1124-1126.

(a)



localized electron pair

(b)



delocalized electron pair



Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Ligand Modification of Ni-Pincer Complexes for Electrochemical H₂ Evolution

Jaewhan Cho, Junhyeok Seo*

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

In today's energy crisis, humans are developing new energy storage systems to convert and store the renewable and sustainable energy sources. Importantly, current air pollution and the global warming issues demand the sustainable and carbon-free methods. Dihydrogen is a simplest energy storage molecule, and the hydrogen-based fuel cell technique and the developed catalytic systems for the $2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$ reaction make its utilization seem promising. As known, platinum is the most efficient single element catalyst for the electrochemical H₂ evolution; however, the precious metal is not appropriate for the mass production process. Thus, catalytic systems based on the low cost and earth-abundant metals are pursued. There exist numerous H₂ generating/splitting catalysts in nature and synthetic systems. The hydrogenases are the essential enzymes in nature, involving metabolism of most of the microbes. In particular, the [FeFe]-hydrogenase active site has been extensively studied in the line of developing H₂-catalysts. One of the key features of the enzyme active site is the flexible amine pendant named azadithiolate, which delivers protons to the Fe active site efficiently. The proton-delivering amine pendant has been also used in the synthetic systems. The known complexes containing amine pendants have shown relatively high overpotentials, or one-directional H₂ splitting or generating reactivity. We are interested to control the direction of the hydrogen reaction, and as well minimize the overpotentials during the proton reduction reaction. For the purpose, we synthesize pincer type complexes possessing the flexible amine pendant, and modify the ligand moiety, and tune the electronic property.

Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

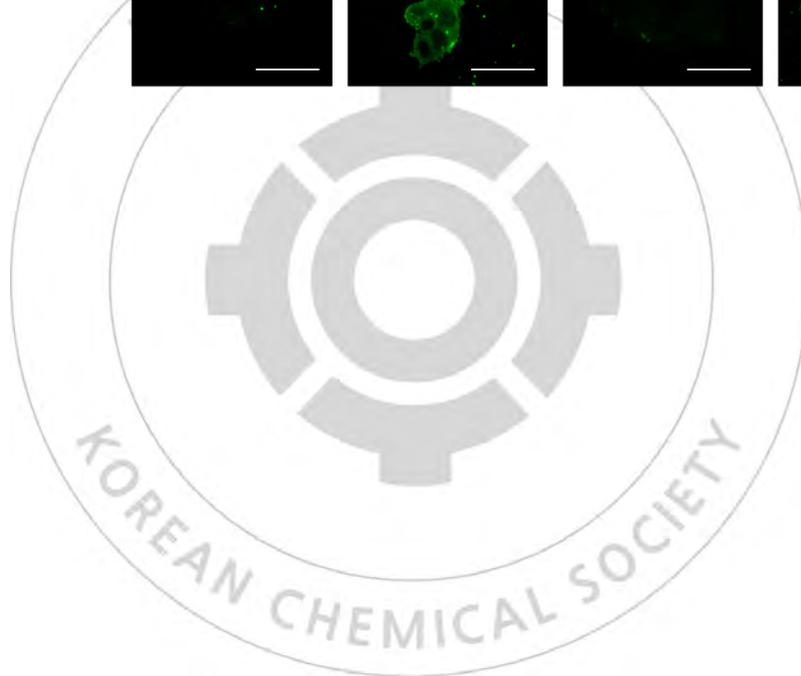
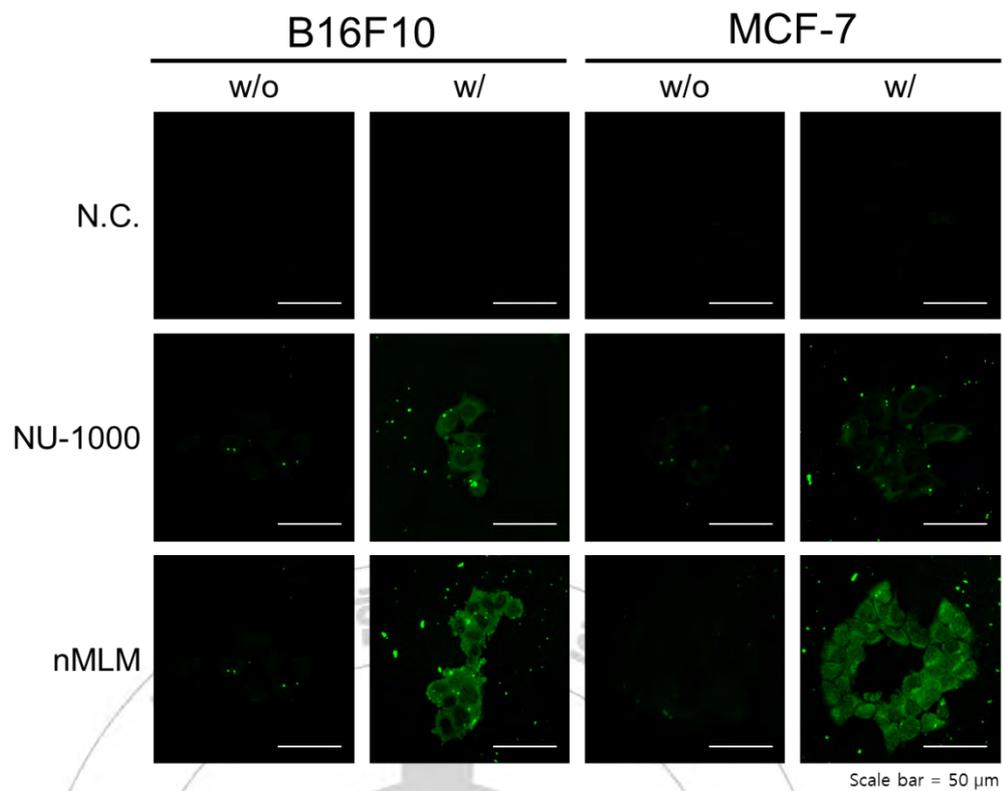
Enhanced Photodynamic Therapy Properties in nano-sized Mixed Ligands Metal-Organic Frameworks

Jiwon Kim, Kyoung Chul Park, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Photodynamic therapy (PDT) is one of cancer treatment methods, which has the merit that minimizes the need for delicate surgery and long-term recovery, and minimizing scar tissue. The PDT application require photosensitizer, light source, and molecular oxygen. The photosensitizer is a chemical compound that can be promoted to an excited state upon absorption of light and undergo intersystem crossing with oxygen to generate highly cytotoxic reactive oxygen species (ROS). Nowadays, many photosensitizers for PDT exist such as porphyrin, BODIPY, phthalocyanine, etc. However, these organic macromolecules have the disadvantage that photosensitizer aggregates in solution because of their hydrophobic properties. Herein, in order to minimise this problem, we synthesized a new type of Zr-based nano-sized mixed-ligand MOFs (nMLMs), which were obtained by the solvothermal reaction between a Zr₆ cluster and a mixture of an appropriate ratio of H4TBAPy and Zn-TCPP. The mixed-ligand strategy successfully yielded MLMs because of the identical symmetry and connectivity of the two ligands. The synthesized nMLM has the advantage of preventing aggregation of photosensitizer due to ordered structure which is an important feature of metal organic frameworks. Moreover, due to complementary absorption and energy transfer between the two ligands in the nMLMs, our nMLMs performed as superior photoinduced reactive oxygen generators, verifying the enhanced light-harvesting properties of the pyrene- and porphyrin-based nMLMs, thereby leading to high photodynamic therapy activity. Fig 1. ROS generation by NU-1000 and nMLM in B16F10 and MCF cells

Acknowledgment : 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- 2016R1A2B4010376).



Poster Presentation : **INOR.P-102**

Inorganic Chemistry

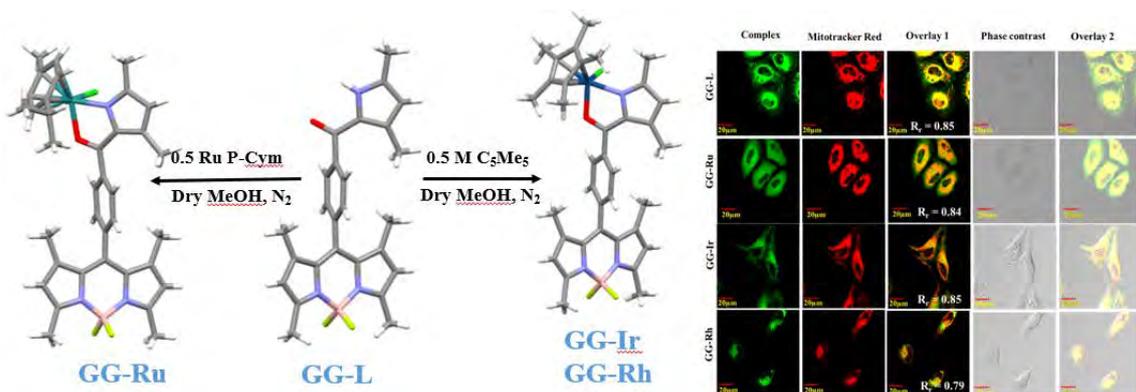
Exhibition Hall 2, THU 11:00~12:30

Highly Photostable Novel BODIPY based Metal Complexes for Mitochondrial Localization

Gajendra Gupta, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Mitochondria, the energy (ATP) producing organelles present in most eukaryotic cells, play important role in the metabolism of lipids and some amino acids, maintenance of redox balance, regulation of respiration and control cell death. Dysfunction of mitochondria causes various neurodegenerative disorders such as Alzheimer's and Parkinson's disease, cancer and diabetes. Thus, tracking mitochondria are essential to further understand the various cellular functions and help in treating mitochondria-related pathologies. Therefore, there is a need for the development of new fluorescent mitochondria selective probes which are photostable and low cytotoxic for live cell imaging. Here, in this study a novel N,O based BODIPY ligand was synthesized and further utilized to develop highly fluorescent and photostable Ru(II), Rh(III) and Ir(III) metal complexes. The complexes are fully characterized by different analytical techniques including single crystal XRD structures. The photostability, as well as live cell imaging of the complexes were performed by confocal microscopy. These complexes specifically localized in mitochondria of live cells and show negligible cytotoxicity at the concentration used for the imaging purpose. They also exhibit high photostability since fluorescence intensity remains more than 50% even after 1800 scans. Figure: Reaction scheme showing the formation of metal complexes and their mitochondrial localization images. Reference: 1. G. Gupta, A. Das, N. B. Ghate, T. Kim, J. Y. Ryu, J. Lee, N. Mandal, C. Y. Lee. Chem. Commun. 2016, 52, 4274-4277; Inorg. Chem. 2017, 56, 4615-4621; Chem. Eur. J. 2017, 23, 17199-17203. Acknowledgement: 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-2016R1A2B4010376, NRF-2018R1D1A1B07045863).



Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Assembling M-porphyrin@ZIF with Carbon Nanofiber for Oxygen Evolution and Hydrogen Evolution reaction Electrocatalyst

Sujee Cho, Miyeon Kim, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

The problem of fossil resource depletion and pollution of the environment have been gradually severe. Therefore, studies are actively conducted to exploit high-density hydrogen as fuel.[1] Hydrogen is considered to be clean energy carrier. The splitting of water into hydrogen and oxygen is a crucial component of a promising renewable energy infrastructure and offers a clean route.[2-3] Transition metal based electrocatalysts are cost-effective alternatives as oxygen evolution reaction (OER) process and are potential candidates for sustainable energy. In this study, we successfully self-assembled zeolitic imidazolate frameworks (ZIF-67) with carbon nanofiber (CNF), which is considered to be a good candidate for oxygen evolution and hydrogen evolution reaction because of its abundance of metal center. Since, ZIF-67 has weak dispersive forces, we have introduced CNF with the feature of high conductivity to help dispersion. The synthesized catalyst was analyzed through various analytical techniques such as BET, XRD and SEM. The catalysts under study showed good OER performance. References: 1) J. Bisquert and S. Giménez, Photoelectrochemical Solar Fuel Production 2018, 41-1042) V. Singh and T. Chatterjee, Recent Research in Science and Technology 2013, 5, 76-783) K. S. Joya, Y. F. Joya, K. Ocakoglu and R. v. d. Krol, Water-splitting catalysis and solar fuel devices., 2013, 52, 10426. Acknowledgment : 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- 2016R1A2B4010376).

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Real-Time Colorimetric Detection of Water in Organic Solvents by Dipolar Dye Incorporated into AlPO₄-5 Nanochannel

Hyeonji Yoo, Hyun Sung Kim^{1,*}

Chemistry, Pukyong National University, Korea

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

Water can have a significant impact on the activity and application of chemicals as well as on the production of chemicals. Accurately and quantitatively detecting trace amounts of water in organic products is critical in environmental monitoring and chemical industry processes to maintain the quality, yield or reliability of the final product. We propose a material that can accurately and rapidly quantify new forms of water by adding a dye with dimethylamine within the AlPO₄-5 channel. This AlPO₄-5 and dye composite material has been used successfully in air as well as in high-sensitivity optical humidity sensing materials in organic solvents. By adding a dye to AlPO₄-5, excellent properties as a humidity sensor can be obtained with high sensitivity to water and short reaction time. We show that these humidity sensitivities are derived from the Brønsted-Lowry point of the AlPO₄-5 channel. When the water molecule enters the AlPO₄-5 channel, the dimethylamine of the bipolar dye is protonated by the Brønsted-Lowry acid site, which changes color by reducing donor-accepter internal-charge transfer in the dipole dye. The benefits of dye encapsulation within the AlPO₄-5 channel have also been demonstrated in terms of stability at various temperatures.

Poster Presentation : **INOR.P-105**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Olefin Epoxidation by Nickel Amidate Complex: Proton Switch in the Ligand Sphere to Control Catalytic Events in the Metal Sphere

Soohyung Kim, Cheal Kim¹, Jaeheung Cho², Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

¹*Seoul National University of Science & Technology, Korea*

²*Emerging Materials Science, DGIST, Korea*

We have recently synthesized a nickel(II) complex of new chelating ligand. Built upon a rigid anilidopyridyl [N,N]-bidentate scaffold and flexible bis(pyridylmethyl)amine tether, the N5-pentadentate ligand here serves as a monoanionic ligand by deprotonation of the amide N-H group upon metallation. Using mCPBA as terminal oxidant, this mononickel complex effects catalytic epoxidation of a wide range of olefinic substrates. A combination of X-ray crystallographic, UV-vis/EPR/NMR spectroscopic, and mechanistic studies with substrate probes and isotope labeling have revealed (i) reactivity control by reversible protonation of the secondary coordination sphere; (ii) involvement of high-valent nickel species as the key intermediate for the oxo-transfer step; (iii) exceptionally high conversion of terminal olefins through this catalytic process. In this presentation will be discussed our venture into new territories beyond the traditional "oxo-wall" (where life still continues).

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Reproducible synthesis of a zeolitic imidazolate framework exhibiting MER topology

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¹Chemistry, Soongsil University, Korea

Zeolitic imidazolate frameworks (ZIFs) are assembled from divalent metal ions and imidazoles via solvothermal reactions. Among known many different types of ZIFs, those having zeolite MER topology (ZIF-mer) are hard to synthesize without particular organic templates such as calixarene. After many trials, we could find a simple and reproducible synthetic method for ZIF-mer using mixed imidazoles (imidazole and 2-methylimidazole) and without particular template. If the ratios between two imidazoles are not optimized, other types of ZIFs such as ZIF-pcb or other mixtures are produced. Here, we present the reaction conditions and analysis results including crystal structures.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Exploration of enzyme-mimicking MOFs for decarboxylation of orotic acid derivatives

Kyungkyou Noh, Jiwon Kim¹, Jongbum Oh¹, Jaheon Kim^{1,*}

Department of ICMC convergence technology, Soongsil University, Korea

¹*Department of Chemistry, Soongsil University, Korea*

MIL-101 has been functionalized with amino acids (Lys, Asp) in order to mimic the catalytic function of orotidine 5'-monophosphate decarboxylase (ODcase). Succinic anhydride as a spacer molecule was covalently attached to MIL-101-NH₂ and in turn, the amino acids were coupled with the carboxylic acid terminal of the spacer molecule. The obtained MOFs were subject to reactions for the decarboxylation of orotic acid functionalized with butyl or cyclohexyl groups. In this presentation, preliminary experimental results and their implied meanings in our exploration will be discussed.

Poster Presentation : **INOR.P-108**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Highly Selective and Durable Photochemical CO₂ Reduction by Mn(I)-based hybrid system (OrgD-[TiO₂]-MnP)

Sunghan Choi, Ju Hyoung Jo, Min Su Choe, 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)₃Br (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 (HCOO⁻ versus CO) that surpass the catalytic activities of the 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 persistently produced HCOO⁻ with a >99% selectivity accompanied by a trace amount of CO; the turnover number (TON_{formate}) reached ~250 after 23 h irradiation. The product selectivity (HCOO⁻/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 at low Mn concentration, the Mn-H monomeric mechanism associated with HCOO⁻ formation is dominant, whereas at high Mn concentration, CO is formed via an Mn-Mn dimer mechanism.

Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Solid-state photochromism from molecular assembly of bis-*o*-carboranyl siloles

Jin-Hyoung Kim, Su-Jin Kwak, Changyun Back, Chul Hoon Kim*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A new type of solid-state photochromism was observed in an AB₂ type molecular assembly comprising the central silole and two peripheral *o*-carborane units, and depending on the assembling positions of those units at adjoining phenyl group two different conformational isomers were formed, namely **Si-*m*-Cb** and **Si-*p*-Cb**. Each isomer showed different solid-state photochromism depending on its solid state morphology, either in the crystalline or amorphous state. Photophysical studies on each isomer in the solid-state revealed that electronic interaction between silole and *o*-carborane units determined emission colors. The crystal and DFT optimized structures each accounting for the crystalline and amorphous structure, respectively, and correlated well to the electronic interaction on the molecular assembly in the solid state, thus enabling to predict solid state morphological change, *vide infra*.

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

An Investigation on Photocatalytic CO₂-to-CO Conversion Activities of Heteroleptic [Ir(C[^]N)₂(N[^]N)]⁺-type Complexes-Sensitized TiO₂ Ternary Hybrids (IrPS/TiO₂/Re(I))

Sunghan Choi, Ju Hyoung Jo, Daehan Lee, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Herein, we report a detailed investigation of efficient hybrid photocatalysts system for carbon dioxide reduction. The system is based on a co-assembly of Ir(III) photosensitizer (Ir-PS) and molecular Re(I) reduction catalyst on TiO₂ semiconductor. The hybrid system consists of cationic iridium(III) complexes [Ir(C[^]N)₂(N[^]N)]⁺ (dfppyIrP, C[^]N = 2-(2,4-difluorophenyl)pyridine (dfppy); ppyIrP, 2-phenylpyridine (ppy); btpIrP, 2-(benzo[b]thiophen-2-yl)pyridine (btp); piqIrP, 1-phenylisoquinoline (piq); N[^]N = 4,4'-X₂-bipyridine (X = CH₂PO(OH)₂)) as a visible-light photosensitizer and fac-[Re(4,4'-bis(methylphosphonic acid)-2,2'-bipyridine)(CO)₃Cl] as a CO₂ reduction catalyst (ReP), both of which have been fixed onto TiO₂ semiconductors (Hombikat-TiO₂). Overall the present Ir(III) complex-based hybrid series showed the most durable, efficient catalytic activities compared to typical homogeneous (Ir-PS + ReP) and our previous binary system (Ir-PS + TiO₂/ReP). Among four ^XIrP-sensitized TiO₂ hybrids, btpIrP/TiO₂/ReP hybrid exhibited the best conversion activity with its relatively higher visible light absorption coverage.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Double *p*-type doping Effects for the Complex Zintl Compounds: $\text{Ca}_{10.88(4)}\text{Li}_{0.12}\text{Sb}_{9.32(1)}\text{Ge}_{0.42(1)}$, $\text{Ca}_{10.94(3)}\text{Na}_{0.06}\text{Sb}_{9.43(1)}\text{Ge}_{0.45(1)}$

JunSu Lee, Tae-Soo You*

Department of Chemistry, Chungbuk National University, Korea

Recently, we reported the multi-substitution effect for the thermoelectric(TE) performance in the $\text{Ca}_{11-x}\text{Yb}_x\text{Sb}_{10-y}\text{Ge}_z$ ($0 \leq x \leq 9$; $0 \leq y \leq 3$; $0 \leq z \leq 3$) system. In this work, we exploited a cationic mixture of Ca/Yb and the *p*-type dopant Ge for Sb and studied their influences for the electronic structures as well as TE performance. As an extension of this study, we present experimental and theoretical investigations using two types of *p*-type dopants in the $\text{Ca}_{11-x}\text{M}_x\text{Sb}_{10-y}\text{Ge}_z$ ($\text{M} = \text{Li, Na}$; $x = 0.06(3), 0.12(4)$; $y = 0.57(1), 0.68(1)$; $z = 0.42(1), 0.45(1)$) system. Here instead of a simple cationic mixture, we also introduced two different monovalent cations, Li and Na, along with the anionic Ge doping. Two title compounds in the $\text{Ca}_{11-x}\text{M}_x\text{Sb}_{10-y}\text{Ge}_z$ system have been synthesized by the high-temperature synthetic method using arc-melting and characterized by both powder and single crystal X-ray diffractions. Two title compounds crystallized in the isotopic crystal structure of the $\text{Ho}_{11}\text{Ge}_{10}$ -type (tetragonal space group $I4/mmm$, Pearson symbol $tI84$) with nine crystallographically independent atomic sites in each unit cell, which include one $\text{Ca}^{2+}/\text{M}^+$ mixed-cationic site and one Sb/Ge mixed-anion site. The overall crystal structure can be described as an assembly of three different types of co-facial polyhedra formed by $\text{Ca}^{2+}/\text{M}^+$, which of each is centered by isolated Sb atoms. Moreover, the three-dimensional anionic skeletons can be considered as an assembly of the dumbbell- and square-shaped Sb atoms. To further understand the overall electronic structure and chemical bonding in the title compounds, a series of DFT calculations using tight-binding linear muffin-tin orbital method were performed for two hypothetical structural models of $\text{Ca}_{10.5}\text{M}_{0.5}\text{Sb}_{9.5}\text{Ge}_{0.5}$ ($\text{M} = \text{Li, Na}$). In addition, the density of states, crystal orbital Hamilton population curves, band structures, and electron localization function were thoroughly interrogated as well.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Analysis of the Visual and Circadian Properties of a Multi-Package Phosphor-Converted LED for Indoor Lightings

Yun Jae Eo, Heejoon Kang, Soomin Ahn, Keyong Lee, Young rag Do*

Department of Applied Chemistry, Kookmin University, Korea

Since the appearance of GaN-based blue light-emitting diodes (LEDs), artificial lighting types, including indoor lightings, have quickly been replaced by LEDs because white light can be easily realized using down-conversion phosphors such as the $Y_3Al_5O_{12}:Ce$ yellow phosphor. However, because modern society has concerns about artificial lighting, researchers have begun to pay attention to the effects of this type of light on the human body, especially on the circadian rhythm, and to the efficiency of different forms of artificial lighting. The circadian rhythm, which affects the secretion and suppression of melatonin, is known to be associated with the intensity of the blue spectral power distribution upon exposure to this type of light. In this study, we fabricated white phosphor-converted LEDs (pc-LEDs) using three types of phosphor materials (red, green and amber) and blue LEDs in order to improve the color rendering index (CRI) and to evaluate the visual and circadian properties of these LEDs. White pc-LEDs were able to realize white light at various correlated color temperatures (CCTs) from 2,000 to 10,000 K when the applied current was adjusted. As a result, the circadian illuminance was found to increase with an increase in the CCT, although the visual illuminance was similar regardless of the CCT. We also found that it is necessary to reduce exposure to blue-enriched white light to decrease the disturbance to the circadian rhythm.

Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Application on Tri-packaged White Down-Converted LEDs using Green Zn-Ag-In-S/Zn-In-S/ZnS for High Color Qualities

Minji Ko, Hyeongjin Lee¹, Young rag Do^{2,*}

Department of Chemistry, Kookmin University, Korea

¹*Department of Applied Chemistry, Kookmin University, Korea*

²*Department of Bionano Chemistry, Kookmin University, Korea*

In this study, we synthesized highly efficient green Zn-Ag-In-S/Zn-In-S/ZnS (ZAIS/ZIS/ZnS) quantum dots (QDs) using a hot-injection method to realize tri-packaged white down-converted light-emitting diodes (DC-LEDs). To improve the photoluminescence quantum yield (PLQY), we added a Zn-In-S inner shell to mitigate the lattice mismatch between the ZAIS alloy core and the ZnS outer shell. The synthesized ZAIS/ZIS/ZnS showed a high PLQY of 0.85 with a peak wavelength of 506 nm. Additionally, we synthesized red Zn-Cu-In-S/ZnS to apply to the tri-packaged white DC-LEDs. The obtained ZCIS/ZnS showed a PLQY of 0.84 with a peak wavelength of 585 nm. We fabricated the obtained green ZAIS/ZIS/ZnS and red ZCIS/ZnS into a cup-type blue InGaN LED. We realized tri-packaged white DC-LEDs at a correlated color temperature (CCT) in the range of 2,700 K to 10,000 K. The tri-packaged white DC-LEDs exhibit a high luminous efficacy (LE) value of 81 lm/W at an applied current of 180 mA, a color rendering index (CRI, Ra) = 90, and external quantum efficiency (EQE) of 0.29 at 5,700 K. As a result, this study indicates that the synthesized QDs would be good candidates for applications involving white DC-LEDs providing high energy performance and ultrahigh color quality levels.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Construction of Rigid Hetero-Multimetallic Co₂Pt₈ Supramolecular Cages Having D₄ Symmetry

Ji Yeon Ryu, Junseong Lee*

Department of Chemistry, Chonnam National University, Korea

Two types of rigid hetero-multimetallic tetragonal prismatic cages were prepared by [2 + 4] stoichiometric reaction of tetrapotic N-donor pyridine (electron donor) and 60° Pt organometallic linker (electron acceptor). The formation of self-assembled cages were characterized by various analytical methods including ¹H, ³¹P{¹H} NMR spectroscopy, electrospray ionization mass spectrometry (TQ-ESI-MS), and elemental analysis. The NMR spectra of the synthesized cages showed the distinct coordination bonds between pyridyl donor and platinum acceptor and the construction of highly symmetric tetragonal prismatic cages. The volume of the inside cavity is about 400 Å³ which was estimated by molecular model using MM2 force-field simulation, suggesting that it can be an attractive molecular container for host-guest chemistry such as encapsulation of small molecules.

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Enhancement of Photoluminescent Quantum Yield of InP/ZnSeS/ZnS/Zr Quantum Dots by using Multi-Functional Ligand

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²*Department of Bionano Chemistry, Kookmin University, Korea*

We modified a method of synthesizing a Zr shell coated with InP/ZnSeS/ZnS quantum dots (QDs) onto synthesized QDs using $\text{Zr}(\text{OCH}_2\text{CH}_2\text{CH}_3)_4$ in order to enhance the photoluminescent quantum yield (PLQY). We used a 2,2-iminodibenzoic acid (IDA), which has two carboxylic groups and one amine group, as a ligand. In the conventional method, only oleic acid and oleylamine, which have only one functional group each, are used as ligands. However, IDA has more functional groups than the ligands of QDs synthesized by the conventional method. The PLQY of the QDs with the multi-functional ligand as used here is increased by a relative amount of 25.5% compared to conventional QDs, *i.e.*, from 58.5% to 73.4%. Although, the full width at half maximum (FWHM) of the QDs with the multi-functional ligand is still narrow at 53 nm and the emission wavelength was shifted from 521 nm to 523 nm, the shift was not as great as that associated with conventional QDs.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Multinuclear nickel(II) complexes with chiral Schiff base ligands

Ume Farwa, Junseong Lee*

Department of Chemistry, Chonnam National University, Pakistan

We report the synthesis of three hierarchical mono, tetra and hexa nuclear Ni complexes with chiral Schiff base chiral ligands (H_3L_1 , H_3L_2). These multinuclear complexes are characterized by IR, EA, ESI-MS, and X-ray single crystal diffraction. Synthesis of metal complexes by the conventional route at room temperature is difficult to understand as compared to the high-temperature hydrothermal synthesis. There are different factors that control the aggregation of metal complexes such as temperature, ligand design, base used, ancillary ligand, and solvent system. But the main factor that controls this process is not known. Due to the ambiguity in the understanding of the governing factor that controls the synthesis of these aggregates the process is referred to as "serendipitous self-assembly". Usefulness of Nickel metal complexes in single molecular-magnetic and synthetic models for metallo-biomolecules has increased interest in their synthesis. We tried to synthesis different nuclearity Ni metal complexes by controlling the ratio of three reactants i.e. metal salt, ancillary ligand and the main ligand (H_3L_1 , H_3L_2) carrying out the reactions at ambient temperature. Mononuclear complex **1** and tetranuclear complex **2** are isolated by using H_3L_1 as main ligand and NaOAc as ancillary ligand. Whereas, hexa-nuclear complex **3** is isolated using H_3L_2 as main ligand and Na_2CO_3 as a source of ancillary ligand.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Cobalt(III) Complexes Containing [ONNO] Type Tetradentate Pyridoxal Ligand for Cycloaddition Reaction of CO₂ and Epoxide

Sam Hwang, Junseong Lee*

Department of Chemistry, Chonnam National University, Korea

New cobalt complexes, Co(pyr₂en)OAc, were synthesized by the reaction of pyridoxal-based SALEN ligand L₁ or L₂ (L₁=N,N'-bis(pyridoxylideneiminato)ethylene) and Co(OAc)₂. The complexes were characterized by various analytical methods including infrared spectroscopy, EA and ESI-MS. Molecular structure of CoL₁(OAc) was confirmed by single crystal X-ray diffraction study. The complex is composed of a cobalt metal center, a tetradentate schiff base ligand, an acetate ion and a DMSO molecules. By the square planar coordination of the ligands and an acetate anion and a DMSO, cobalt metal center has octahedral geometry. The synthesized cobalt complexes were used for the coupling of CO₂ with epoxides. Co(pyr₂en)OAc showed high activities even in low catalyst loading (0.5mol%-). Various cyclic carbonate were efficiently synthesized from the Co catalysts by changing epoxides.

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Fabrication of a ripple-less narrow bandwidth stop filter with an aperiodic deposition by simulating and depositing a nano-multilayer

Gang Yeol Yoo, JoongHo Lee¹, SeungJae Lee¹, Joo Won Yang², Woong Kim^{3,*}, Young rag Do^{4,*}

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¹*Kookmin University, Korea*

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We introduced ripple-less narrow-bandwidth stop filter (NBSF) with red, green, and blue (RGB) colors by simulating and aperiodic materials deposition with a high refractive index and a low refractive index in an alternating approach. These RGB NBSFs, fabricated by aperiodically depositing low-index SiO₂ and high-index TiO₂, were initially simulated using an “OpenFilters” simulation to fabricate the NBSF and using the “Essential Macleod” software to eliminate unwanted secondary reflections. By adjusting the process by which to eliminate ripples, the simulated reflectance and color coordinates of NBSF were enhanced in the simulated data. The full width at half maximum (FWHM) of the simulated reflectance of the ripple-less RGB NBSF was approximately 50 nm, and the corresponding simulated reflectance exceeded 92% apart from the bandwidth wavelength. From the simulated data, we fabricated a ripple-less RGB NBSF by aperiodically depositing SiO₂ and a TiO₂ nanolayer. The structural properties of the RGB NBSF were examined using transmission electron microscope measurements with a focused ion beam (FIB) in slice mode to confirm coincidence with the simulated data. The optical properties of the RGB NBSF were studied by means of reflectance and transmittance spectroscopy.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Color-by-Blue Three-Package White LED with Narrow-Band BaMgAl₁₀O₁₇:Eu,Mn Green Phosphor and K₂SiF₆:Mn Red Phosphor for a Wide Color Gamut of LED Backlighting Achieves the NTSC Standard of 109.

Heejoon Kang, Tae Gun Kim¹, Keyong Lee², Young rag Do*

Department of Bionano Chemistry, Kookmin University, Korea

¹*Department of Applied Chemistry, Kookmin University, Korea*

²*Kookmin University, Korea*

We introduced narrow-band BaMgAl₁₀O₁₇:Eu,Mn (BAM:Eu,Mn) green phosphors that can be applied as backlighting for liquid crystal displays (LCDs) and can be used with vacuum ultraviolet (VUV) phosphors used only in PDPs due to their high stability. This phosphor absorbs blue wavelength light and can co-dope two types of activator with a broad bandgap of the host material. To meet the requirements of BAM:Eu,Mn phosphors for LED applications, the energy transfer from the absorbed blue energy of Eu²⁺ to the Mn²⁺ ions should be maximized by optimizing the concentrations of both Eu²⁺ and Mn²⁺ ions. Finally, the photoluminescence (PL) emission of the narrow-band green light of the Mn²⁺ activator should be improved by optimizing the blue absorption, blue energy transfer, and green emission characteristics. In this presentation, we demonstrate how BAM phosphors may be a sufficient candidate group for LCD green phosphors and show that a white LED using green BAM and red K₂SiF₆:Mn⁴⁺ (KSF) phosphors is capable of a NTSC ratio efficiency of 109%. Hence, it could be confirmed that these phosphors are feasible for use as a backlighting component of LCDs.

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design of a flexible MOF having catalytic sites and its structural effects on CO₂ cycloaddition reaction

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

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

Flexible metal-organic frameworks (*flex*MOFs) have evolved into a key part of MOF chemistry owing to their responsive character upon external stimuli by altering the pore structures. When this feature is applied to catalyst materials, it will versatily control their pore size for guest molecules, leading to catalytic efficiency and selectivity. Although *flex*MOFs could be expected to show an interesting performance on catalytic reactions, few studies have been conducted so far. In this work, we designed a new flexible MOF, *flex*MOF(CN), with dangling nitrile groups, which can coordinate active transition metals as a single-site catalyst. Therefore, we prepared *flex*MOF(CN)-Co(II) by post-synthetic metalation, which retains the same flexible behaviors as *flex*MOF(CN). *flex*MOF(CN)-Co(II) was utilized in a cycloaddition reaction of CO₂ with epoxides. As a result, *flex*MOF(CN)-Co(II) showed a great performance for various types of epoxide substances by responsively changing its pore structure upon a size of substances.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Reduce mustard gas simulant by using ZIF-8(Zeolitic Imidazole Framework)

Son Yerim, Hyun Sung Kim^{1,*}

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

When people exposed by mustard gas, get serious burn damage and injury and leftover of gas effect by carcinogen to DNA, it cause mutation of gene. The gas is prohibited internationally because it can cause large and continuous damage to a wide range at once, but the manufacturing is cheap and simple, and there is a risk to use it in terrorist organizations such as IS. In experiment, mustard gas is too dangerous, so we use simulant of Mustard Gas, CEES(Chloroethyl ethyl sulfide).ZIF-8(Zeolitic Imidazole Framework) is consisted with Zirconium and imidazolate ligand. Structure of ZIF-8 is similar to Architecture of zeolite, but Si is replaced by Metal and O atoms are replaced by imidazolates. Like Zeolite, ZIF-8 have Porous structure and inside of pore is hydrophobic which mean capture organic matters, like toluene, well. Our purpose is using ZIF-8's zeolitic porous structure and property of holding organic matter, capturing or decompose CEES.Through experiments, we have confirmed that ZIF-8 adsorbs CEES well . also has attempted to produce better and more stable adsorption / decomposition catalysts by changing the metal or ligand in ZIF-8.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Electromagnetic interference shielding of Nonwetting Flexible Free- Standing MXene-Carbon Fabric composite

Kyu Yun Chai*, **Leero Lee¹**, **Sohyeon Kim¹**, **Seung Yu Choi¹**, **Hasu Jung²**

Department of Chemistry, Wonkwang University, Korea

¹*Wonkwang University, Korea*

²*Organic Chemistry, Wonkwang University, Korea*

The nonwoven carbon fabric and are an excellent candidate for electromagnetic interference(EMI) shielding. using X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM), mapping, and Raman spectroscopy characterization have been done for the composite. The hydrophobic MXene-carbon fabric composite posses contact angle of 123° with spreading coefficient of -112.66 mN/m, wetting energy of -39.86 mN/m and work of adhesion 32.94 mN/m. The thermally stable composite prevents the degradation of up to 235 °C. The composite pertaining excellent electric conductivity of 8.5 S/cm with 6.5 Ω/sq of sheet resistance. 43.2 dB of maximum EMI shielding exhibited at 2.3 GHz with 8534.7 dB cm²g⁻¹ of absolute shielding effect. The composite can be utilized for various application areas such as portable electronics, military, aviation, aerospace and radars

Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Electromagnetic Shielding of water repellent Lightweight and Flexible Graphene-Coated Fabric compost and MXene-Graphene-PVDF Composite foam

Kyu Yun Chai^{*}, Youngee Park¹, Keunhwa Kim¹, Subin Oh¹

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¹*Wonkwang University, Korea*

The spray coating and solvent casting strategy were used to prepare MXene and graphene-based thin, flexible and low-density composite. The crystallinity, morphology, elemental analysis and bonding nature have been analyzed by using X-ray diffraction (XRD), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray (EDX) and Raman spectroscopy. The composite exhibited maximum electric conductivity of 13.68 S cm⁻¹ with 3.1 Ω/sq of lowest sheet resistance. The hydrophobic composite exhibited a maximum of 126 ° with spreading Coefficient of -116 mN/m, wetting energy of -43 mN/m and lowest work of adhesion of 30 mN/m. The composites displayed outstanding thermal stability and inhibit the thermal degradation up to 400 °C. The maximum EMI shielding of 53.8 dB (99.999 %) exhibited in the X-band region by MXene-graphene foam with dominant absorption of 43.38 dB and 13.10 dB of reflection. The exceptional absolute shielding effectiveness of 35,369.82 dBcm²g⁻¹ showed by single coated graphene-carbon fabric. The above outcomes outlook application areas such as mobile phones, handy electronics, aeronautics, air travels, radars and soldierly applications.

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Hydrogen Bond-Enabled Heterolytic and Homolytic Peroxide Activation within Nonheme Copper(II)-Alkylperoxo Complexes

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¹*Department of Chemistry, Sookmyung Women's University, Korea*

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-125**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Curvature-dependent Growth behaviors of Zincone MLD Film on Nanostructured Surfaces

Hyemi Lee, Jin seok Lee^{1,*}

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¹*Department of Chemistry, Sookmyung Women's University, Korea*

Molecular layer deposition (MLD) is a method for obtaining conformal ultrathin organic films using vapor-phase organic precursors, while their composition and thickness can be controlled at the molecular level. This MLD process is based on self-limited reactions between the precursors and the substrate surface. Also, in comparison with solution-based technique, it allows epitaxial growth of molecular layer on substrate, and is especially good for surface reaction or coating of nanostructures such as nanopore, nanobead, nanowire array and so on. In this study, we fabricated organic-inorganic zincone polymeric films on surfaces with various curvatures through coupling reactions between diethyl zinc (DEZ) and diol with triple bonds as inorganic and organic precursors, respectively, by molecular layer deposition. Using ellipsometry and transmission electron microscope (TEM) analysis, we characterized the different growth behavior of zincone films grown on curved substrates, and demonstrated the curvature-dependent growth mechanism of MLD film on nanostructured surfaces. Reference[1] J. S. Lee, Y. -J. Lee, E. L. Tae, Y. S. Park, K. B. Yoon, *Science*, 2003, 301, 818–821.[2] A. A. Dameron, D. Seghete; B. B. Burton, S. D. Davidson, A. S. Cavanagh, J. A. Bertrand, S. M. George, *Chem. Mater.* 2008, 20, 3315–3326.[3] A. I. Abdulagatov, R. A. Hall, J. L. Sutherland, B. H. Lee, A. S. Cavanagh, S. M. George, *Chem. Mater.* 2012, 24, 2854–2863.[4] Y.-S. Park, S.-E. Choi, H. Kim, J. S. Lee*, *ACS Applied Materials & Interfaces*, 2016, 8 (18), 11788–11795.[5] Y.-S. Park, H. Kim, B. Cho, C. Lee, S.-E. Choi, M. M. Sung, J. S. Lee*, *ACS Applied Materials & Interfaces*, 2016, 8 (27), 17489–17498.

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Elucidating the Mechanism of Atomic Layer Deposition in Solution Using Germanium and Antimony Precursors with Tellurium Reagent

JeongMin Hwang, Bo Keun Park, Taek-Mo Chung^{1,*}

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea

¹*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

This study suggested that the elucidation of relationship between steric hindrance of alkoxy carbon of aminoalkoxide ligands and formation of telluride materials such as germanium telluride (GeTe) and antimony telluride (Sb₂Te₃). To demonstrate such phenomena, we prepared germanium precursors, Ge(dmamp)₂, Ge(dmap)₂, and Ge(dmae)₂, along with antimony precursors, Sb(dmamp)₃, Sb(dmap)₃, and Sb(dmae)₃ using various aminoalkoxide ligands with different alpha carbon substituent group, dmampH, dmapH, and dmaeH. Prepared complexes were further treated with bis(trimethylsilyl)tellurium in hexadecane through thermal decomposition reaction and the resultants were studied with powder X-ray diffraction to compare the formation of germanium telluride (GeTe) and antimony telluride (Sb₂Te₃) alloys. After thermal decomposition, Ge(dmamp)₂ and Sb(dmamp)₃, having most bulky substituent group, were transferred into only metallic germanium and antimony. On the other hand, the resultant materials from dmapH and dmaeH, less steric hindrance, revealed rhombohedral phase of GeTe and tellurium or rhombohedral phase of Sb₂Te₃ and tellurium. These results suggested that the formation of chalcogenide alloy is more favorable when relatively less bulky ligand was used.

Poster Presentation : **INOR.P-127**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis, Crystal Structures, and Characterization of Three New Metal Organic Coordination Polymers, $[(TC)_6Zn_3(bipy)]$, $[(TC)_6Co_3(bipy)]$ and $[(TC)_4Cu_2(bipy)]$

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Chemistry, Chung-Ang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

Metal organic coordination polymers (MOCs) of $[(TC)_6Zn_3(bipy)]$ (**1**), $[(TC)_6Co_3(bipy)]$ (**2**) and $[(TC)_4Cu_2(bipy)]$ (**3**) (*bipy* = 4,4'-bipyridine and *TC* = 3-thiophenecarboxylate) were synthesized by hydrothermal reactions. Single crystal X-ray diffraction indicated that compounds **1** and **2** were crystallized in the triclinic space group, *P*-1 (No. 2). The two compounds are isostructural to each other. Compound **3** crystallized in the monoclinic space group, *P*2₁/*c* (No.14). All of the reported compounds reveal infinite 1D chain structures. In particular, compounds **1** and **2** reveal peddle wheel-like structures and compound **3** exhibits a ladder-like structure. *TC* ligands are coordinated to the metal cations (Zn^{2+} , Cd^{2+} , and Cu^{2+}) and form clusters that are connected each other by *bipy* ligands as organic linkers. Compounds **1**, **2**, and **3** were characterized by powder X-ray diffraction, IR spectroscopy, thermogravimetric analysis (TGA), elemental analysis (EA), UV-Vis diffuse reflectance spectrum, photoluminescence (**1**), and direct-current magnetic susceptibility (**2**).

Poster Presentation : **INOR.P-128**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

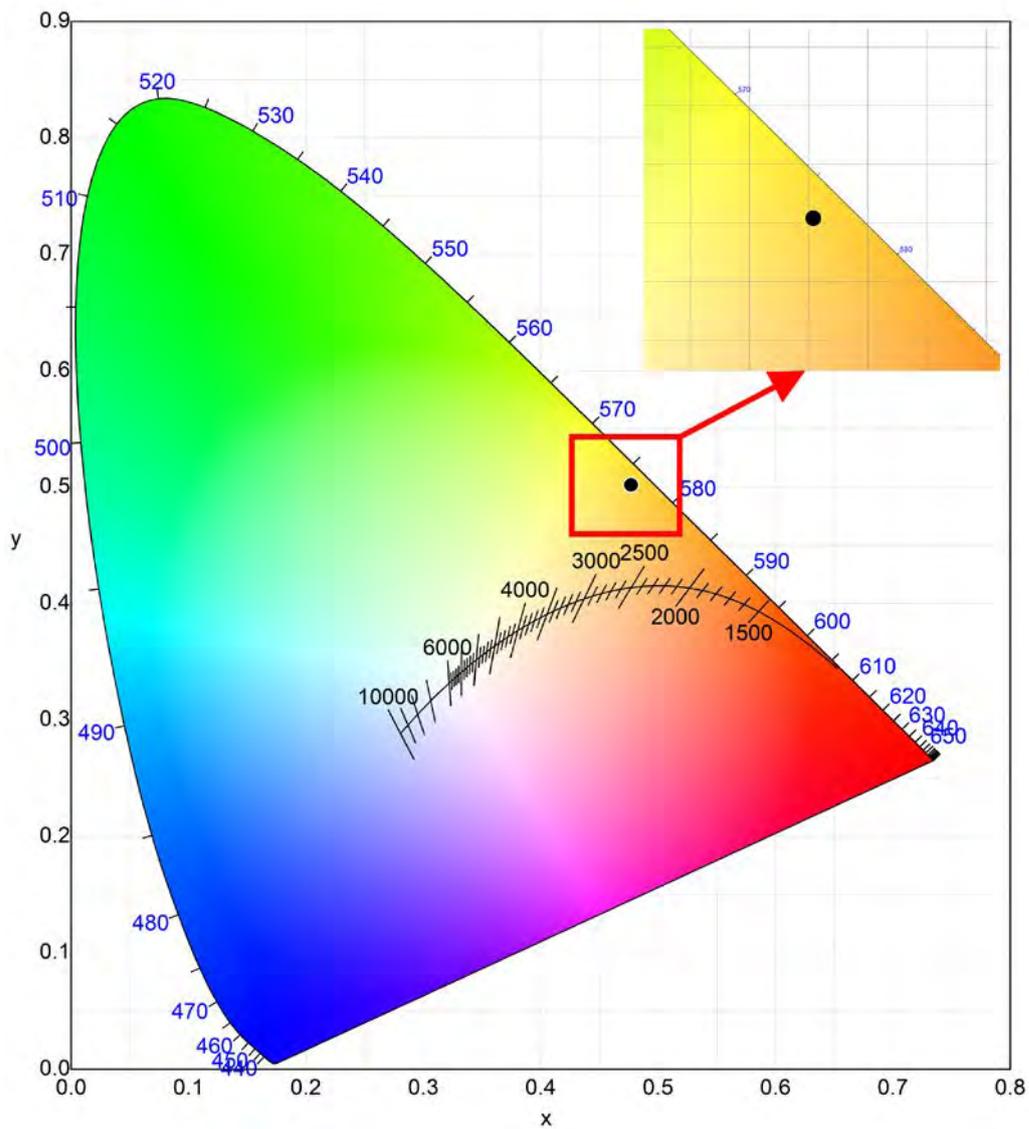
New Antimony-Based Chiral Organic–Inorganic Hybrid Materials with Yellow Photoluminescence

TaeHwan Moon, Kang Min Ok^{1,*}

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¹*Department of Chemistry, Sogang University, Korea*

In recent years, organic-inorganic hybrid materials are of great interest due to their remarkable optoelectronic properties. Therefore, various applications such as photodetectors, photocatalysts, and light-emitting diodes are being applied. Among many, chiral lead halides containing chiral organic molecules with pseudo-perovskite materials have also exhibited interesting photovoltaic applications including ferroelectricity and photoluminescence (PL). However, toxic lead is harmful to the environment and the human body. We have synthesized new organic-inorganic hybrid materials using less toxic antimony and chiral organic amines. The new organic-inorganic hybrid chloroantimonates(III) composed of (R)/(S)-1-phenylethylammonium cation were synthesized using a solution process technique. Single crystal X-ray diffraction analysis confirms that both R- and S- configuration hybrids were crystallized. Both compounds crystallized in the polar space group, $P2_1$. While the R-configuration compound shows the unit cell parameters of $a = 12.161(2) \text{ \AA}$, $b = 12.883(3) \text{ \AA}$, $c = 15.098(3) \text{ \AA}$, and $\beta = 101.87(3)^\circ$, those for the S-configuration compound are $a = 11.954(2) \text{ \AA}$, $b = 12.835(3) \text{ \AA}$, $c = 14.892(3) \text{ \AA}$, and $\beta = 101.30(3)^\circ$. PL measurements revealed that the synthesized materials reveal yellowish light. The CIE chromaticity coordinate calculated based on the emission spectrum of the R-configuration compound indicates that the material is located in the yellow region with the coordinate (0.48, 0.50). Full characterization including IR spectra, UV-vis reflectance spectra, thermogravimetric analysis, and powder X-ray diffraction are also presented.



KOREAN CHEMICAL SOCIETY

Poster Presentation : **INOR.P-129**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis, structure, and characterization of new lanthanoid tellurium oxide nitrate compounds, $M(\text{TeO}_3)(\text{NO}_3)$ ($M=\text{Y}$, La , and Eu)

HyeEun Lee, Kang Min Ok^{1,*}

Department of Chemistry, Chung-Ang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

A series of novel lanthanoid tellurium oxide nitrate compounds, $M(\text{TeO}_3)(\text{NO}_3)$ ($M = \text{Y}$, La , and Eu) were synthesized in a closed system in the absence of water. The crystal structures of the reported materials were determined by powder and single-crystal X-ray diffraction. $M1(\text{TeO}_3)(\text{NO}_3)$ ($M1 = \text{Y}$ and Eu) reveals a two-dimensional (2D) layered structure that crystallizes in the centrosymmetric orthorhombic space group, *Cmca* (No. 64). $M2(\text{TeO}_3)(\text{NO}_3)$ ($M2 = \text{La}$) also exhibits a two-dimensional (2D) framework structure crystallizing in the monoclinic space group, *P2₁/n* (No. 14). The novel compounds were completely characterized by infrared and UV-vis diffuse-reflectance spectroscopies, thermogravimetric analysis (TGA), energy dispersive X-ray spectroscopy (EDS), bond valence sum calculations, and photoluminescence (PL) measurements.

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

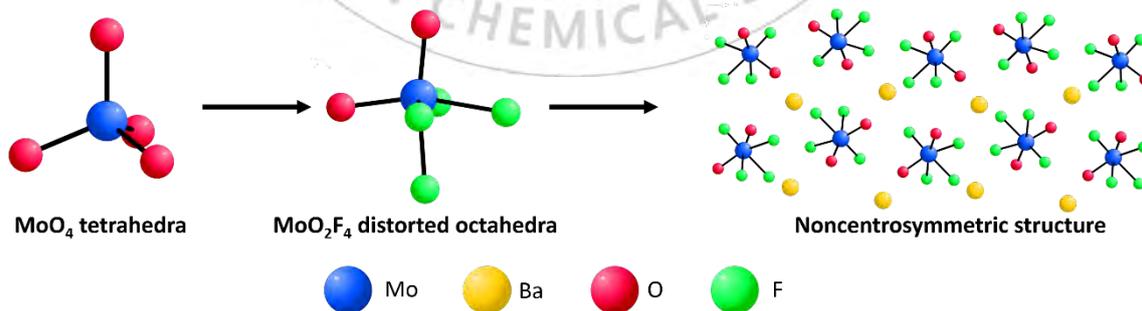
A new noncentrosymmetric molybdenum oxyfluoride

Hongil Jo, Kang Min Ok^{1,*}

Department of Chemistry, Chung-Ang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

When Mo^{6+} cation is in a six-coordinate environment with oxide ligand, it forms an octahedral geometry with the off-centered distortion. If the asymmetric units align in parallel manner, the crystal structure loses the center of symmetry and has a net polarization. Unfortunately, Mo^{6+} tends to form four-coordinate geometry which is undesirable to macroscopic noncentrosymmetric (NCS) structure. In this research, fluoride was used to prevent four-coordinate geometry. By doing so, we have successfully synthesized a novel NCS alkaline earth metal molybdenum oxyfluoride. Single crystal X-ray diffraction indicates that the title compound crystallizes in the polar orthorhombic space group, $Pca2_1$. The asymmetric unit of the compound is composed of Ba^{2+} and $[\text{MoO}_2\text{F}_4]^{2-}$ ion. Local dipole moment calculations indicate that the net polarization of the compound is due to the alignment of $[\text{MoO}_2\text{F}_4]^{2-}$ ion. Further characterizations such as spectroscopic analysis and thermal analysis are also presented.



Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

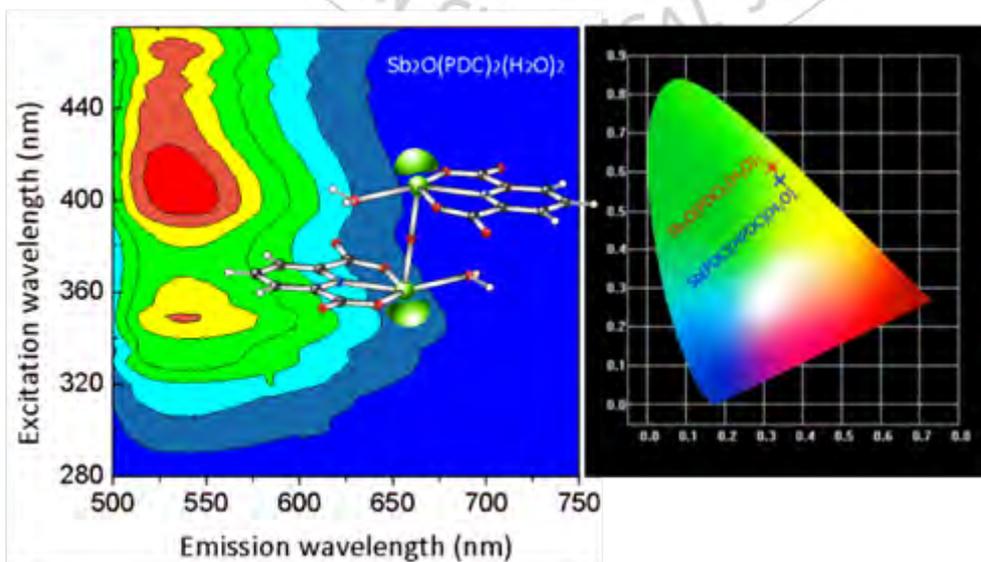
Sb(III)-Coordination Complexes Exhibiting Yellowish Green Emissions with Outstanding Lifetimes

Haixin Qi, Kang Min Ok^{1,*}

Department of Chemistry, Chung-Ang University, Korea

¹Department of Chemistry, Sogang University, Korea

Two antimony(III)-based coordination complexes, $\text{Sb}(\text{PDC})(\text{HPDC})(\text{H}_2\text{O})$ and $\text{Sb}_2\text{O}(\text{PDC})_2(\text{H}_2\text{O})_2$ (PDC = pyridine-2,6-dicarboxylate) have been synthesized via hydrothermal reactions. Single-crystal X-ray diffraction indicates that $\text{Sb}(\text{PDC})(\text{HPDC})(\text{H}_2\text{O})$ and $\text{Sb}_2\text{O}(\text{PDC})_2(\text{H}_2\text{O})_2$ are composed of SbO_3N_2 or SbO_4N polyhedra, 2,6-PDC ligand, and H_2O . The central Sb(III) cations in both materials are in highly distorted environment attributable to the stereoactive lone pairs on Sb(III) ions. UV-vis diffuse reflectance spectra clearly indicate that the introduction of Sb(III) cations into the coordination system through the red-shift of the maximum peaks. Photoluminescence measurements suggest that $\text{Sb}_2\text{O}(\text{PDC})_2(\text{H}_2\text{O})_2$ is a single component yellowish green light emitting material with a remarkable decay lifetime of 8.4 μs at room temperature.



Poster Presentation : **INOR.P-132**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Two New Transition Metal fluorides with Dimeric and Monomeric Asymmetric Basic Building Units

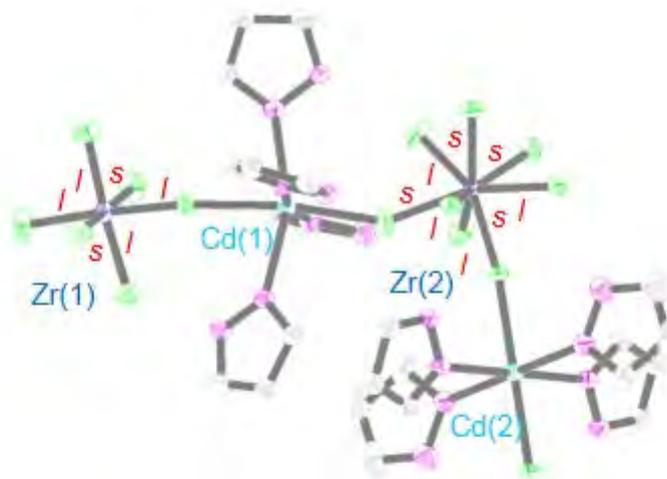
Belal Ahmed, Kang Min Ok^{1,*}

Department of Chemistry, Chung-Ang University, Korea

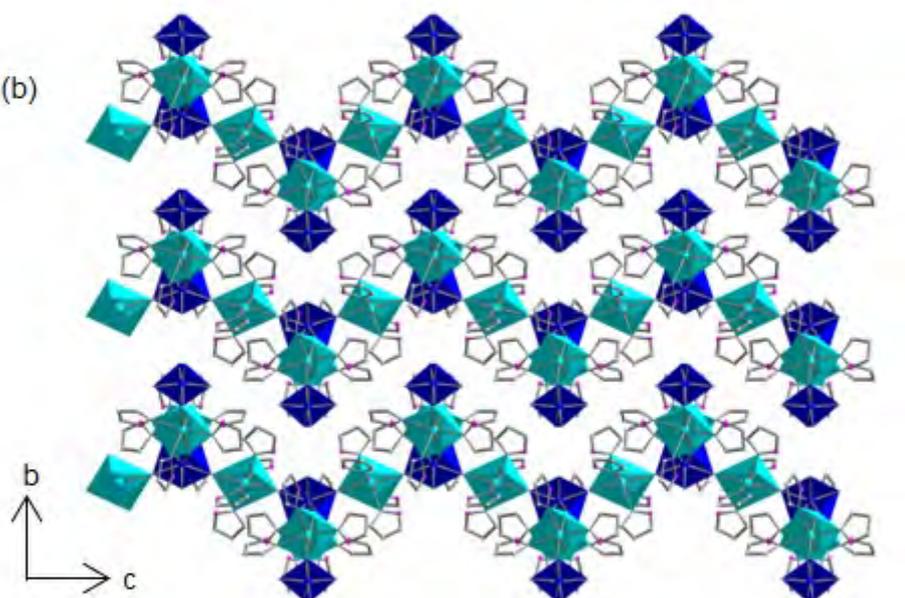
¹*Department of Chemistry, Sogang University, Korea*

Two new transition metal fluorides revealing two-dimensional layered zigzag chain structures composed of asymmetric basic building units of dimeric $[\text{Zr}_2\text{F}_{12}]^{4-}$ /monomeric $[\text{ZrF}_6]^{2-}$ and $[\text{ZrF}_8]^{2-}$ polyhedra, and polarizable LTM cations (Zn^{2+} and Cd^{2+}), and heterocyclic ligands [pyrazole (pz) and 3-methylpyrazole (mpz)], i.e., $[\text{Zn}(\text{mpz})_3][\text{ZrF}_6]$ (**1**), $[\text{Cd}(\text{pz})_4]_3[\text{ZrF}_6][\text{ZrF}_8]$ (**2**), have been synthesized via hydrothermal reactions. Compounds **1** and **2** crystallize in the monoclinic crystal space group, $P21/c$ and $P2/c$, respectively. Careful structural analysis suggests that the distinctive structure-directing anionic groups and hydrogen bonding interactions are responsible for the zigzag chain structures. Both of the title compounds show higher-energy absorption band gaps ranging from 4.38 to 4.47 eV, which originate from the distortion of M^{2+} cations in octahedral geometry, and electronic transitions between the valence and conduction band edges comprised of filled d^{10} orbitals and empty d^0 orbitals. The reported compounds have been also thoroughly characterized using spectroscopic and thermal analyses along with calculations of local dipole moments and the extent of out-of-center distortions.

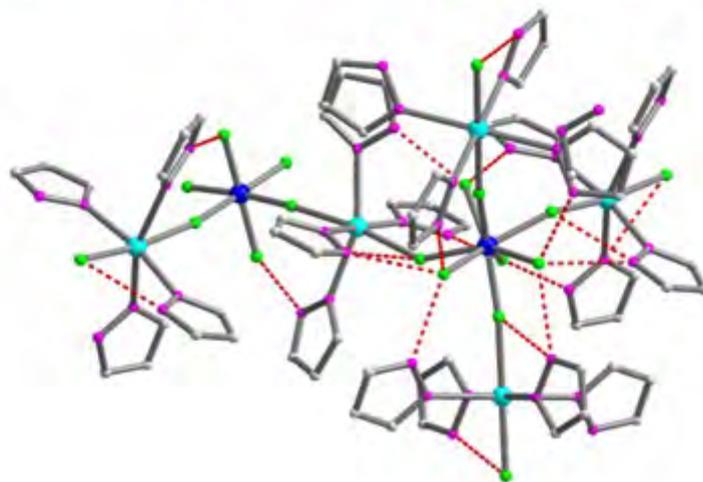
(a)



(b)



(c)



Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Structure and Phase Transition of Polyoxoperoxomolybdates

Jiyeon Hwang, Kang Min Ok^{1,*}

Chung-Ang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

Four novel polyoxomolybdates (POMo), $\text{Cs}_5[\text{Na}(\text{H}_2\text{O})_5][\text{Mo}_7\text{O}_{24}]\cdot\text{H}_2\text{O}$ (**Cs-0**), $\text{Cs}_5[\text{Na}(\text{H}_2\text{O})_5][\text{Mo}_7(\text{O}_2)\text{O}_{23}]\cdot\text{H}_2\text{O}$ (**Cs-1**), $\text{Cs}_4[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]\cdot\text{H}_2\text{O}$ (**Cs-2**), and $\text{Cs}_4[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]\cdot 2\text{H}_2\text{O}$ (**Cs-3**), have been synthesized through a slow evaporation method. Among the title compounds, **Cs-1**, **Cs-2**, and **Cs-3** are polyoxoperoxomolybdates (POPOMo) including peroxo ligands in the metal-oxide cluster. The reported compounds were characterized by X-ray diffraction, infrared spectroscopy, and thermogravimetric analysis. **Cs-0**, **Cs-1**, and **Cs-2** crystallize in the triclinic space group, *P*-1, while **Cs-3** crystallizes in the monoclinic space group, *C2/m*. Both **Cs-0** and **Cs-1** consist of Cs^+ cations, $\text{Na}(\text{H}_2\text{O})_5$, and polyoxyanion clusters, $[\text{Mo}_7\text{O}_{24}]^{6-}$ and $[\text{Mo}_7(\text{O}_2)\text{O}_{23}]^{6-}$, while **Cs-2** and **Cs-3** consist of Cs^+ cations and $[\text{Mo}_4(\text{O}_2)_2\text{O}_{12}]^{4-}$ polyoxyanions. The oxidation states of the molybdenum cations in all the reported compounds are +6. A phase transition of metal-oxide cluster was monitored during the solution evaporation. Further studies to explain the transition mechanism of the title compounds are in progress.

Poster Presentation : **INOR.P-134**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Hydrothermal Synthesis and Characterization of a Cesium Niobium Oxyfluoride

Hyeshin Lee, Kang Min Ok^{1,*}

Department of Chemistry, Chung-Ang University, Korea

¹Department of Chemistry, Sogang University, Korea

A new cesium niobium oxyfluoride, $\text{Cs}_{30}\text{F}_{85}\text{Nb}_{19}\text{O}_{22} \cdot 2\text{H}_2\text{O}$ has been synthesized by a hydrothermal reaction in the presence of HF solution. The synthesis of the material has been adjusted by varying the amount of fluoride. Single crystal X-ray diffraction indicates that the title material crystallizes in the trigonal space group, $P\bar{3}m$. The scanning electron microscope (SEM) image reveals that the morphology of the material is hexagonal. Also, the ratio of heavy elements, i.e., Cs:Nb detected by energy-dispersive X-ray spectroscopy (EDX) is approximately 3:2. In the structure, water molecule is surrounded by polyhedra of niobium and cesium cations. Moreover, by the measurement of powder X-ray diffraction with increasing temperature, it has shown that the material has a good thermal stability up to 400 °C. Ion exchange experiments of cesium cations for other alkali metal cations are in progress.

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Rb₇MY₂B₁₅O₃₀ (M = Sr and Ba): Two New Rare-earth Borates as Potential Ultraviolet Nonlinear Optical Materials

Xinglong Chen, Kang Min Ok^{1,*}

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

¹*Department of Chemistry, Sogang University, Korea*

Two new rare-earth borate crystals, Rb₇MY₂B₁₅O₃₀ (M = Sr and Ba), have been synthesized by a high-temperature solution method and their structures were determined by single crystal X-ray diffraction. The two compounds are isostructural with the noncentrosymmetric space group, R32. In their structures, the B₅O₁₀ clusters are connected by the YO₆ octahedra forming an intricate three-dimensional [Y₂(B₅O₁₀)₃]⁹⁻ anionic architecture, and the Rb⁺ and M²⁺ (Sr²⁺ or Ba²⁺) cations fill into the cavities to keep the charge balance. Experimental studies show that the two compounds possess relatively large second harmonic generation (SHG) responses (~1.1 and 1.2 × KH₂PO₄ at 1064 nm, respectively) with phase-matching abilities. Importantly, the title materials display short cutoff edges below 190 nm. Moreover, first-principle theoretical studies were carried out to obtain better understanding of the structure-property relationships. Both experimental and theoretical studies suggest that Rb₇MY₂B₁₅O₃₀ (M = Sr and Ba) are potential nonlinear optical materials for UV applications.

Poster Presentation : **INOR.P-136**

Inorganic Chemistry

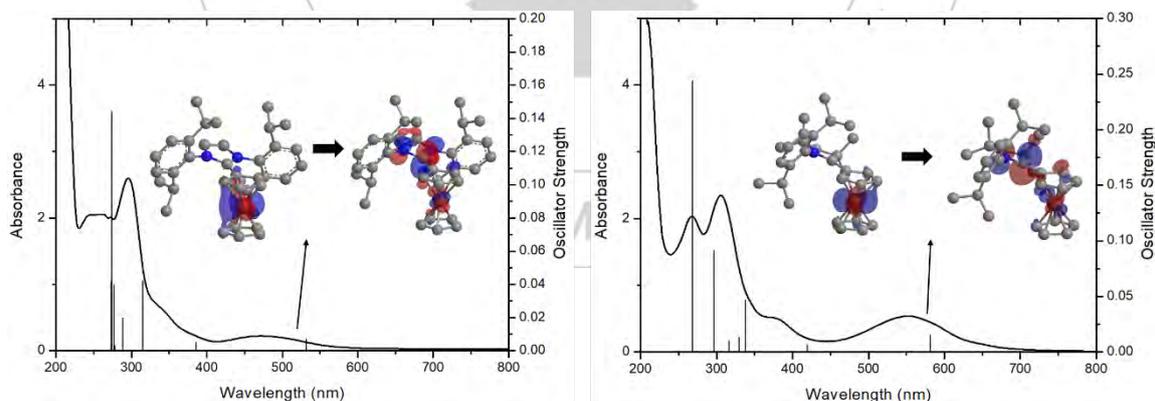
Exhibition Hall 2, THU 11:00~12:30

***N*-heterocyclic Carbene (NHC)-functionalized Ferrocene Cation: Synthesis, Spectroscopic and Computational Studies**

Hayoung Song, Eunsung Lee*

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

We could successfully characterize the reactivity between NHC and ferrocenium to afford NHC-functionalized ferrocene. The NHC-functionalized ferrocene complex shows the strong metal-to-ligand charge transfer (MLCT) bands. These MLCT bands are strongly depended on the electrophilicity of NHCs. Thus, cyclic (alkyl)(amino)carbene (cAAC)-functionalized ferrocene cation shows red-shifted absorption band compared to imidazolium-functionalized ferrocene. Furthermore, the NHC-functionalized ferrocene cation can be applied to one-electron reduction to afford NHC-stabilized Fe(I)-ferrocene.



Poster Presentation : **INOR.P-137**

Inorganic Chemistry

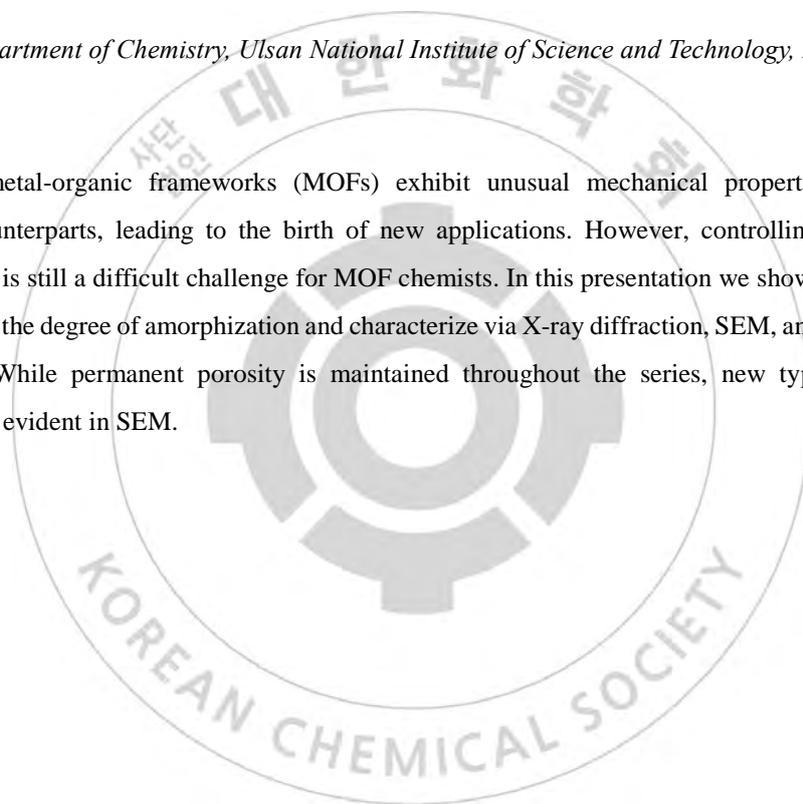
Exhibition Hall 2, THU 11:00~12:30

Controlling Amorphization in Metal-Organic Frameworks

Joohan Nam, Eunji Jin, Wonyoung Choe*

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

Amorphous metal-organic frameworks (MOFs) exhibit unusual mechanical properties unlike their crystalline counterparts, leading to the birth of new applications. However, controlling the degree of amorphization is still a difficult challenge for MOF chemists. In this presentation we show a new series of MOFs varying the degree of amorphization and characterize via X-ray diffraction, SEM, and gas adsorption experiments. While permanent porosity is maintained throughout the series, new type of core-shell morphology is evident in SEM.



Poster Presentation : **INOR.P-138**

Inorganic Chemistry

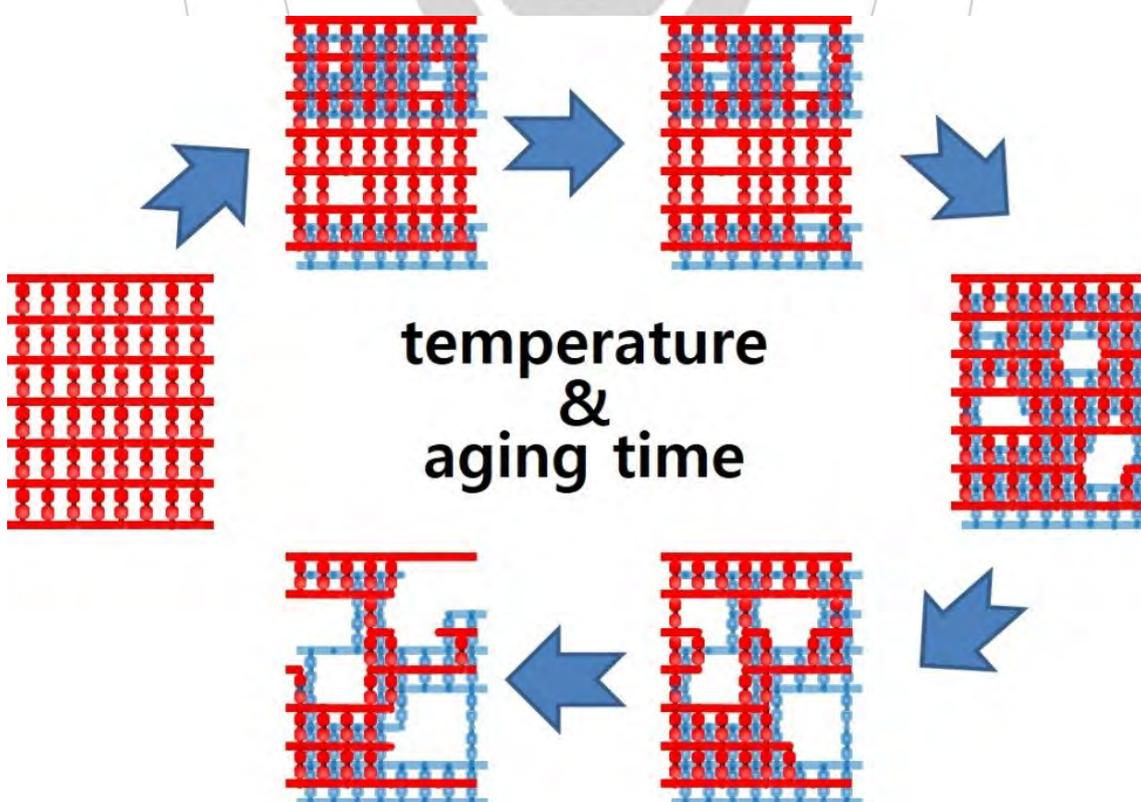
Exhibition Hall 2, THU 11:00~12:30

Control of micro- and meso-porosity in metal-organic frameworks

Seok Jeong, Myoung Soo Lah*

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

Non-interpenetrated three-dimensional metal-organic framework (MOF) with hms topology is converted to doubly interpenetrated analogues with hms-c topology by thermal treatment. Depending on thermal treatment condition and the property of the neutral pillaring linker, the defects of the MOFs can be potentially controlled. Combination of non-stoichiometric removal of neutral pillaring linkers from MOFs and partial collapse of two-dimensional sheets could lead to new hierarchically porous interpenetrated MOFs that contain both micro- and mesopores simultaneously.



Poster Presentation : **INOR.P-139**

Inorganic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Enhancement of selective heavy metal adsorption ability due to amino acid in MOF-808

Junmo Seong, Myoung Soo Lah*, Seungwan Han

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

N-Acethyl-L-cysteine (AcC)-grafted MOF-808 was prepared by exchanging formates at Zr metal centers of MOF-808 exposed in the solvent pore. Since MOF-808 has six formates per $Zr_6O_4(OH)_4$ cluster, N-Acethyl-L-cysteine with thiol residue can be introduced into the pore up to six molecules by exchanging formate with N-Acethyl-L-cysteine. The amount of N-Acethyl-L-cysteine molecules was confirmed by NMR and the presence of thiol group was confirmed by FT-IR. Heavy metal adsorption process of AcC-grafted MOF-808 followed pseudo 2nd order kinetic model. AcC-grafted MOF-808 showed 95.9% removal of Cd^{2+} and its K_d value is 2.31×10^4 , which is moderate compared to other porous systems. The maximum uptake of Cd^{2+} was 225.1 mg/g, which is the highest value among MOF systems. In addition, AcC-grafted MOF-808 showed excellent selectivity for Cd^{2+} and Pb^{2+} over other alkali and transition metal ions.

Poster Presentation : **PHYS.P-76**

Physical Chemistry

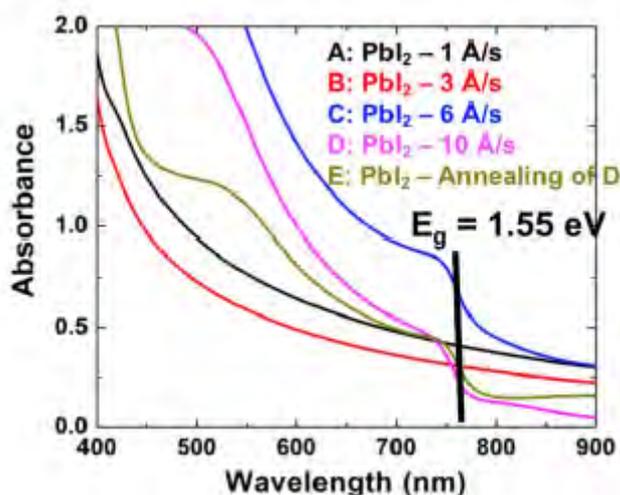
Exhibition Hall 2, FRI 11:00~12:30

Observation of intermediate state in organic-inorganic hybrid perovskite thin film fabricated by two-step sequential vacuum evaporation method

Young Mi Lee

Beamline Department, Pohang Accelerator Laboratory (PAL), Korea

Organic-inorganic hybrid perovskites (OHP), described by ABX_3 (A = organic cation, B = metal cation, X = halogen anion) has attracted much attention as a candidate material for future solar-cell applications with easy-fabrication, low-cost, and high-efficiency. Therefore, OHP materials are motivated not only to enhance performance for solar-cell application but also to bring to light new phenomena relevant to other technological application such as light emitting diode, laser, optoelectronics and thermos electronics, among others. We performed the systematic experiment with different inorganic material first layer deposition rates to confirm the quality of thin films fabricated by the sequential vacuum evaporation method (SVE) method. As the deposition rate was increased, the hybrid perovskite forms well. However, we found the tiny grain and the intermediate state, and the molecular defect is observed. From these findings, we speculate why a vacuumevaporated OHP-based solar-cell has relatively low PCE and material instability.



Poster Presentation : **PHYS.P-77**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Implementation of the method of separable solution for Hartree-like equations by Teller and Sahlin's variation method to obtain directly the threshold wavefunctions for Rydberg series $n\ell$ of many electron diatomic molecules

Chun-Woo Lee

Department of Chemistry, Ajou University, Korea

Unified treatment of molecular photoabsorption and photoionization requires the analytical continuation of quantum defects of bound excited state wavefunctions into the phase shifts in continuum wavefunctions across the threshold. In multichannel quantum defect theory, the energy insensitive nature of quantum defects is utilized to achieve the analytical continuation. In the past, threshold quantum defects are obtained by extrapolating the solutions at highly excited states calculated by the quantum chemical method, which requires a huge number of basis functions and thus computationally very demanding. On the other hand, direct calculation of threshold solutions was attempted long ago by Hellmig for the separable differential equations in spheroidal coordinates in one-electron diatomic molecules. His method, however, cannot be applied to many electron molecules. Teller and Sahlin used variation method to extend the applicability of the method using separable equations in spheroidal coordinates to many electron molecules. The variation equations thus obtained were considered too complicated to solve directly. Fitting to the experimental data was employed, instead. Although this semiempirical method proved rather successful, its application to obtain threshold solutions by Hellmig's method is found to be problematic. I thus resort to the original variation equation. Its implementation turns out to be not impossible although not so simple. Its implementation and application to HeH^+ are reported here.

Poster Presentation : **PHYS.P-78**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication of porous gold nanoshells *via* nanosecond-laser irradiation

Tae-Hyeon Park, Du-Jeon Jang*

Department of Chemistry, Seoul National University, Korea

Needs for new synthetic methods to fabricate diverse gold nanostructures have increased rapidly. In addition to wet-chemical synthesis, pulse-laser irradiation can be a promising approach to fabricate gold nanostructures with unique morphologies and superior properties to meet the needs. Indeed, controlled heating of gold nanostructures with a laser in the femtosecond or picosecond regime has been developed with detailed calculations. In the meantime, nanosecond lasers have been exploited in limited ways due to their slow pulse duration times, which make the controlled heating difficult. Here, we demonstrate a use of a nanosecond laser to acquire desired gold nanostructures. With the help of silica nanotemplates, hollow and porous gold nanoshells (HPA NSs) were fabricated *via* pulse-laser irradiation. The synthetic strategy mainly relies on the surface melting of gold nanoparticles induced by nanosecond-laser irradiation. Bonds among the gold nanoparticles are formed following the surface melting, and the bonds make it possible for the gold nanostructures to preserve their structure after the removal of the silica nanotemplates. The HPA NSs exhibited high SERS efficiency for the detection of methylene blue due to their high surface area. Thus, we consider that HPA NSs fabricated *via* laser irradiation can be utilized for the detection of molecules, and our synthetic strategy suggests a new extensibility of nanosecond lasers for the fabrication of gold nanostructures with unique morphologies.

Poster Presentation : **PHYS.P-79**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile fabrication of silver nanoparticle arrays by optical-induced melting and dewetting of silver paste

Joon Ki Kim, Tae-Hyeon Park, Dong-Won Jeong, Zee Hwan Kim, Du-Jeon Jang*

Department of Chemistry, Seoul National University, Korea

Highly dense plasmonic silver nanoparticle (NP) arrays have been fabricated by laser-induced dewetting of commercially available silver paste as a starting bulk material. Laser-irradiation criteria for the laser melting, dewetting, and ablation of silver paste films have been determined in order to understand the optimal conditions of laser fabrication. The first laser-scan mode has produced unprecedented intermediate structures, so called laser-induced fine silver nanostructures (LIFSs) while the second laser-scan mode has transformed LIFSs into plasmonic silver NP arrays via the dewetting of the priorly formed nanostructures. The laser-induced fabrication of silver NP arrays has been found to be very sensitive to distance from secondly irradiated laser pulses, suggesting that the fine control of laser intensity is very important. Silver NP arrays of sub-100 nm diameters with narrow size distribution have been fabricated well at a laser scanning rate of $\geq 50 \mu\text{m/s}$. As-prepared silver NP arrays have generated numerous hot spots to show highly strong surface-enhanced Raman scattering signals; the Raman enhancement factor of silver NP arrays for rhodamine 6G has been found as 1.2×10^6 . Overall, our fabrication method of plasmonic silver NP arrays via laser-induced dewetting is facile, scalable, and reproducible.

Poster Presentation : **PHYS.P-80**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Stepwise growth of CdS quantum dots in ethylene glycol

Dong-Won Jeong, Du-Jeon Jang*

Department of Chemistry, Seoul National University, Korea

Colloidal quantum dots (QDs), which have size-dependent band-gap energies with remarkably high quantum yields, have received great attentions. Those intriguing properties are related to the surface states of QDs. Therefore, controlling the surface structure of QDs has been of big importance and varying the types of ligands has been often attempted as means of surface control. Water-dispersive CdS quantum dots have been rapidly synthesized in a polyol solvent of ethylene glycol at 160 °C without using nonpolar organic solvents and their stepwise growth mechanisms have been investigated thoroughly. CdO and 3-mercaptopropionate ions react in water to form cadmium thiolate complexes, which transform gradually into CdS QDs in ethylene glycol at 160 °C. Absorption spectra reveal that the growth rate of CdS QDs in the first step of ≤ 70 s is noticeably faster than that in the second step of ≥ 70 s. Static and time-resolved PL spectra suggest that the dominant growth mechanism of CdS QDs switches from the OR growth in the first step to the OA growth in the second step. PL decay profiles have suggested that the fast decay time of 40 ns and the slow decay time of 300 ns are due to the decay times of excitons in internal defects (IDs) and OA-induced defects (OADs), respectively. In the first step, IDs are eliminated by the OR growth to reduce PL and the center of the PL of the slow decay component shifts from 550 nm to 600 nm as ligands dissociate to leave sulfur atoms on the surfaces of CdS QDs. In the second step, the OA growth occurs to enhance the number of OADs, increasing PL at 600 nm. Overall, the two stepwise mechanisms of the OR growth and the OA growth can be well distinguishable in a polyol solvent of ethylene glycol at a high reaction temperature of 160 °C.

Poster Presentation : **PHYS.P-81**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Hydrothermal fabrication of porous ZnS photocatalysts with a controlled amount of S vacancies

SooHo Ham, Du-Jeon Jang*

Department of Chemistry, Seoul National University, Korea

2D Porous nanostructures have advantages like a high surface area, and high charge transfer rate for photocatalytic applications. In spite of these advantages, the applications of 2D porous nanostructures have been restricted because of complicate fabrication processes. To overcome the drawback, we have fabricated barbell-shaped porous ZnS nanostructures via a thermal decomposition of organic-inorganic hybrid precursor templates ($\text{ZnS} \cdot (\text{ethylenediamine}, \text{en})_{0.5}$). Through the hydrothermal reaction of $\text{ZnS} \cdot (\text{en})_{0.5}$, volatile en molecules has been eliminated to form porous ZnS nanostructures. The thermal transformation of nanocomposites causes crystal defects due to the rearrangement of atoms. These crystal defects can have both positive and negative effects on photocatalytic activity because the defect energy levels can separate excited charges or can act as the recombination sites of excited charges. Thus, controlling the surface defects is an important work to increase photocatalytic activities. During the hydrothermal treatments, it is possible to control the amount of S vacancies by varying the hydrothermal treatment time. The concentration of S vacancies have been estimated by measuring XPS spectra and photoluminescence (PL) spectra from S vacancies of porous ZnS nanostructures. When applied to photocatalytic RhB degradation, porous ZnS prepared by hydrothermal treatment for 4 h have exhibited 8.2 times higher photocatalytic activity than commercial ZnS. Overall, the facile hydrothermal treatment of $\text{ZnS} \cdot (\text{en})_{0.5}$ has increased photocatalytic activities by forming surface sulfur vacancies, which lead to the separation of excited charges.

Poster Presentation : **PHYS.P-82**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Oxidative Degradation of Refractory Contaminants Mediated by Surface $\text{SO}_4^{\cdot-}$ Immobilized on Metal Oxides

Yun Jeong Choe, Sang Hoon Kim, Jongsik Kim*

Materials Architecturing Research Center, Korea Institute of Science and Technology, Korea

$\cdot\text{OH}$ has been regarded as one of potent oxidants to degrade aqueous pollutants, yet, oftentimes remains challenging in terms of its proficient utilization as a recalcitrants' consumer. This is because of 1) a short lifetime of $\cdot\text{OH}$ active in decomposing pollutants under a narrow pH span, 2) a limited quantity of H_2O_2 activators ($\text{M}^{\delta+}$, M: metal; $\delta \leq 2$) to form $\cdot\text{OH}$, 3) oxidation of $\text{M}^{\delta+}$ species to form M^{3+} analogues sluggish to dissect H_2O_2 , and 4) severe leaching of $\text{M}^{\delta+}$ species to catalyze H_2O_2 scission via heterogeneous catalysis. In contrast, $\text{SO}_4^{\cdot-}$ was reported to provide several benefits relative to $\cdot\text{OH}$ such as 1) a longer lifetime and 2) a greater oxidation ability over a wide pH range, yet, could not be free from serious leaching of $\text{S}_2\text{O}_8^{\cdot-}$ activators ($\text{M}^{\delta+}$) to form $\text{SO}_4^{\cdot-}$ species used to oxidize aqueous contaminants. This presentation highlights an adaptable synthetic method of SO_4^{2-} -functionalized metal oxide platforms to sustain the degradation of contaminants via unique heterogeneous catalytic pathway. Specifically, both $\text{M}^{\delta+}$ and SO_4^{2-} species are populated on the surfaces of metal oxides, wherein $\text{M}^{\delta+}$ species catalytically cleave aqueous H_2O_2 to produce $\cdot\text{OH}$, whereas SO_4^{2-} functionalities are excited by radicals from aqueous $\cdot\text{OH}$ species and thus are transformed into surface $\text{SO}_4^{\cdot-}$ species. This presentation also showcases kinetic analysis on a series of controlled reaction runs. This was used to conclude 1) ' $\text{H}_2\text{O}_2 \leftrightarrow \cdot\text{OH} \leftrightarrow \text{SO}_4^{2-} \leftrightarrow \text{SO}_4^{\cdot-}$ ' pathway' is greatly feasible and 2) 'surface $\text{SO}_4^{\cdot-}$ species' are 'major' active sites to consume pollutants with great activity and 'recyclability' via 'heterogeneous catalysis'.

Poster Presentation : **PHYS.P-83**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhancement of visible to UV up-conversion response of hollow phosphor $\text{Y}_2\text{SiO}_5:\text{Pr}^{3+}$ by using surface plasmon resonance.

Edgardo Gabriel Santoro, Young soo Kang^{1,*}

Sogang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

Phosphor up-conversion materials (UCM) $\text{Y}_2\text{SiO}_5:\text{Pr}^{3+}$ (YSO: Pr^{3+}) can do wavelength conversion of visible light into UV light.[1] However, the main constrain about these types of materials is a low conversion efficiency, this limits their applications. The surface plasmon resonance (SPR) effect by using silver nanoparticles (NPs) is possible to enhance the luminescence intensity of UCM by incorporation of the hollow sphere between SPR nanoparticle and phosphor layer.[2] Silver nanoparticles with different sizes and SPR wavelength for the absorption of the visible range were prepared, encapsulated by glucose sphere and used it as hard template. For the synthesis of the hollow material, a layer of YOHCO_3 using a urea precipitation and a layer of SiO_2 through the Stöber method were added over the Ag NP template. The final hollow structure was obtained by a heat treatment of 1000 oC for 3 h induced it by the Kirkendall effect.[3,4] The whole structure size was around 300 nm depending on the metal core size. For each phosphor material with different Ag NP core size, an emission spectra were obtained and compared to the emission spectra of YSO: Pr^{3+} , to quantify the enhancement by using SPR and select the optimal conditions to have the highest intensity.

Poster Presentation : **PHYS.P-84**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

CO₂ Activation and Reduction with Nafion/g-C₃N₄/CuInS₂ Photocathode in Photoelectrochemical System

Ignasia Handipta Mahardika, Young soo Kang^{1,*}

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¹*Department of Chemistry, Sogang University, Korea*

Research on the reduction of carbon dioxide has been studied with various methods like photoelectrochemical cells (PEC), but the energy conversion efficiency level obtained is remained still as low. Therefore, the methods for reducing carbon dioxide will be developed with a system which contains several steps [1]. The (040)-BiVO₄ facet engineered photoanode has shown the successful result to improved charge carrier mobility and high photocatalytic active sites for solar light energy conversion [2]. CuInS₂ (CIS) polycrystalline chalcopyrite p-type semiconductor is a photocathode material which has a high photocurrent and tunable conduction band position for CO₂ reduction into liquid solar fuels [3]. The research will begin by developing CuInS₂ (CIS) thin film for photocathode material and modified by the g-C₃N₄ nano-sheet catalyst to act as a reduction potential tuning and the combination of g-C₃N₄ with Nafion to do multiple proton-coupled multiple electron transfer reaction for CO₂ reduction. An electron can be generated from photocatalyst and then stored instantly in a 2D conducting polymer, g-C₃N₄, which sequentially can be transported to a carbon dioxide reduction site. BiVO₄ was also used as a photoanode material which has a function to produce many electrons and protons by water splitting reaction. Moreover, a one-pot reaction is conducting to react the activated carbon dioxide with proton which has been generated from water oxidation. The one-pot reaction is chosen as a strategy to improve reaction efficiency and produce large yields. This reaction is expected to produce ethanol as the final product. Further, the mechanism and analysis study are continued to understand and prove that this system will give a selected product.

Poster Presentation : **PHYS.P-85**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Preparation of Nd₂Fe₁₄B/FeCo Magnetic Nanocomposite by Using Sol-Gel Method

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Nd₂Fe₁₄B/FeCo magnetic nanocomposite was synthesized by using sol-gel method. In detail, as-synthesized cobalt ferrite nanoparticles with size 5 nm were produced by using organic surfactants to modify the surface property of inorganic seed particles. These particles surface was then modified from hydrophobic to hydrophilic by using cetyltrimethylammonium bromide (CTAB). The modified nanoparticles were dispersed into a solution contained NdCl₃, FeCl₃, H₃BO₃, citric acid and ethylene glycol to form a gel mixture at 90 oC. The gel was ignited at 200 oC, then forming oxide form at 800 oC, following by a reduction with CaH₂ to form the composite. The crystal structure of the magnetic materials was characterized by XRD and TEM. The magnetic properties of the magnetic materials was characterized with vibrating sample magnetometer (VSM). The preliminary results showed a sharp decrease in coercivity and remanence as the cobalt ferrite ratio increased.

Poster Presentation : **PHYS.P-86**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photocatalytic properties of ZnO/ZnTe heterostructured film on a FTO substrate for Photoelectrochemical CO₂ reduction

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¹*Department of Chemistry, Sogang University, Korea*

CO₂ conversion into liquid fuels is one of the most important strategies to solve the global energy problems and the environmental global warming caused by green-house gases. Photoelectrochemical(PEC) CO₂ reduction suggests an ideal pathway to produce carbon-based fuels from CO₂ conversion using sunlight [1]. The development of new photocatalytic materials for the CO₂ conversion in PEC system is the most important challenge to get highly hydrocarbon liquid product. Zinc telluride, ZnTe, has attracted considerable attention by including many desired properties promising semiconductor photocathode with a direct band gap of 2.26 eV to utilize solar light effectively [2]. In this study, we report the catalytic properties of zinc oxide nanorod covered with zinc telluride ZnO/ZnTe) as photocathode for CO₂ reduction. ZnO/ZnTe film was fabricated fluorine doped tin oxide (FTO) substrate by anion exchange reactions based on the difference of solubility product constants (K_{sp}) for ZnO and ZnTe. The morphology, structure, optical and electrochemical properties of ZnO/ZnTe photocathode were investigated by scanning electron microscope, x-ray photoelectron spectroscopy, ultraviolet-visible spectroscopy, linear sweep voltammetry, chronoamperometry and electrochemical impedance spectroscopy. CO₂ reduction reaction with ZnO/ZnTe photocathode was performed using BiVO₄ photoanode in PEC system and was obtained formaldehyde and ethanol as major product.

Poster Presentation : **PHYS.P-87**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Tetragonal to Cubic Phase Transition on the Upconversion Luminescence Properties of A/B site Erbium-doped Perovskite BaTiO₃

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Along with the growing number of applications of upconversion materials, the more thorough understanding of their intrinsic mechanisms for the optical processes are required. Thus far, various lanthanides have been investigated and they are considered the representative upconversion system owing to the huge advantage as the optical probes. When it comes to the upconversion energetics and the associated upconversion paths, the role of the host materials is very important, because they provide microscopic environments, in other words, unique lattice structure of the crystalline samples. Generally, the upconversion quantum efficiency is very low (< 1 %) due to the weak transition dipole moment in the 4f-4f forbidden transition. The low quantum yield can be overcome by adjusting the composition of the lanthanide ions and by varying the types of host materials. In this poster, we reported our remarkable finding that the host material, barium titanate (BaTiO₃, BT), the upconversion luminescence efficiency changed as a function of temperature (65 – 155 °C). This was attributed to the phase transition from tetragonal to cubic structures of BT, which was corroborated by high-temperature XRD (X-ray diffraction) measurements. XRD analysis revealed that the high-yield formation of tetragonal barium titanates at room temperature and the phase transition of BT at ~120°C. Furthermore, it turns out that the temperature dependent upconversion luminescence depended on the sites of doping of Er³⁺ at A (Ba²⁺) or B (Ti⁴⁺) in barium titanate, which was explained in terms of symmetry of crystal structure surrounding the Er³⁺ ions.

Poster Presentation : **PHYS.P-88**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Trans-activator of transcription peptide coated ultrasmall Gd₂O₃ nanoparticles

Shuwen Liu, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, China

Gadolinium oxide nanoparticles are extremely useful for biomedical applications because they possess various excellent physical properties which is applicable to cancer theragnosis. In this study, we prepared gadolinium oxide coated with trans-activator of transcription through one-pot process. We characterized the particle size, surface coating structure, relaxivities an in vitro toxicities of the TAT-GNPs. The average particle diameter is obtained to be 1.5 nm. The r_1 and r_2 values of the TAT-GNP are 18.2 and 30.2 s⁻¹mM⁻¹ ($r_2/r_1=1.6$). The in vivo T₁ MR images exhibited positively (or T₁) enhanced contrasts in the mouse liver cancer after intravenous administration, demonstrating that the TAT-GNPs acted as an enhanced cancer-imaging agent similar to the cancer-targeting agent in T₁ MR imaging (T₁ MRI).

Poster Presentation : **PHYS.P-89**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Study of various sizes of Polyacrylic acid (PAA) coating ultrasmall Gd₂O₃ nanoparticles for MRI

Xu Miao, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, China

Magnetic resonance imaging has become a powerful tool for diagnosis due to the valuable researches on the MRI contrast agents. For biomedical application MRI-CAs nanoparticle should be stable, highly water soluble, non-toxic, and ultrasmall in particle size. In this work, we used different size of water soluble and biocompatible ligand for the surface coating of the nanoparticles. The different ligands size effect on the spin water proton relaxation were observed. They were characterized by HRTEM, XRD, FT-IR, TGA, Cytotoxicity and Map image. The nanoparticles were found monodisperse and average particle diameter is estimated to be ~2 nm. And non-toxic for biomedical application.



Poster Presentation : **PHYS.P-90**

Physical Chemistry

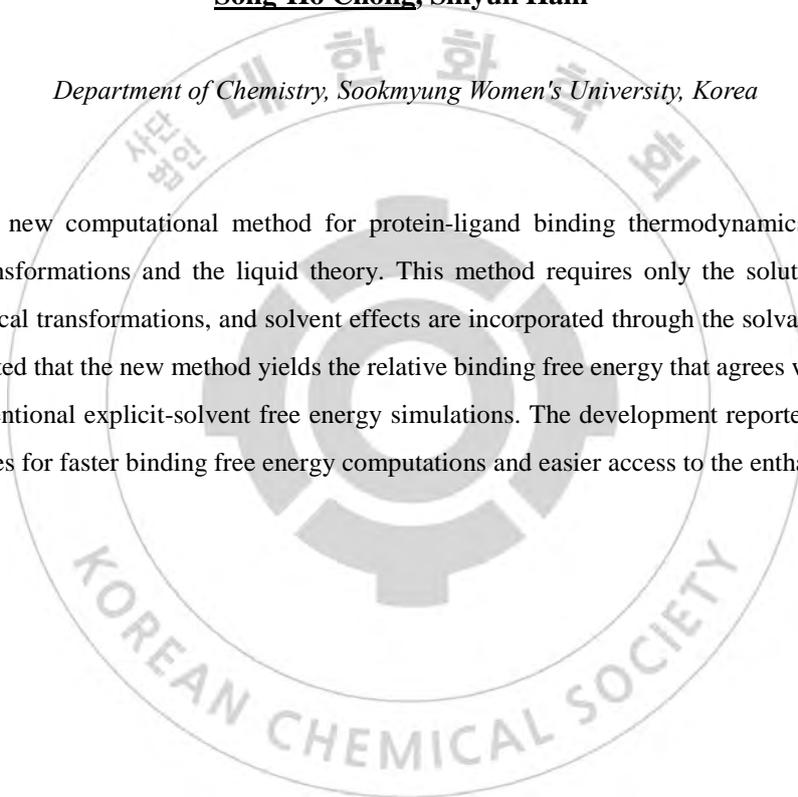
Exhibition Hall 2, FRI 11:00~12:30

A New Computational Method for Protein-Ligand Binding Thermodynamics

Song-Ho Chong, Sihyun Ham*

Department of Chemistry, Sookmyung Women's University, Korea

We develop a new computational method for protein-ligand binding thermodynamics that combines alchemical transformations and the liquid theory. This method requires only the solute configurations during alchemical transformations, and solvent effects are incorporated through the solvation free energy. It is demonstrated that the new method yields the relative binding free energy that agrees well with the one from the conventional explicit-solvent free energy simulations. The development reported here opens up new possibilities for faster binding free energy computations and easier access to the enthalpy and entropy components.



Poster Presentation : **PHYS.P-91**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Water Soluble Polyacrylic acid Coated Tb₂O₃ Nanoparticles as Dual Imaging Agent: T₂ MRI-Fluorescence Imaging Agent

Shanti Marasini, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Nepal

Surface modification of nanoparticles with multifunctional hydrophilic polymer has been proved as a major achievement in synthesis of highly colloidal and biocompatible magnetic nanoparticles. These polymers render magnetic nanoparticles more stable, water soluble and uniform which makes it easier for post synthesis modification and functionalization for bio-applications such as drug delivery, magnetic resonance imaging, cell targeting and hyperthermia. Here, we present the synthesis of ultrasmall Terbium oxide nanoparticles coated with water soluble and biocompatible Polyacrylic acid (PAA~1800 gm/mol) using polyol method. Nanoparticles were characterized by measuring their particle diameter, hydrodynamic diameter, surface coating, magnetic moment (M), r_1 and r_2 values, map images, and in vitro cellular toxicity using different characterization techniques. The fluorescence property was studied through photoluminescence spectrometry and confocal laser scanning microscopy. In vivo MR images were recorded which shows the negative contrast enhancement on liver and kidney after 15 minutes of injection. Hence it can be inferred that ultrasmall Tb₂O₃ nanoparticles can be used as T₂-FI imaging agent.

Poster Presentation : **PHYS.P-92**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

X-ray Attenuation Properties of Ultrasmall Yb₂O₃ Nanoparticles as a High-Performance CT Contrast Agent

Adibehalsadat Ghazanfari, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Iran

Ultrasmall heavy metal-oxide nanoparticles can be utilized for highly enhancing contrasts in computed tomography (CT). In this study, ultrasmall Yb₂O₃ nanoparticles coated with biocompatible and hydrophilic D-glucuronic acid were for the first time prepared through a simple one-step polyol process, and their X-ray attenuation properties were investigated by measuring phantom images and X-ray attenuation powers. The average particle diameter of the nanoparticles was estimated to be 2.1 ± 0.1 nm by using transmission electron microscopy. The observed X-ray attenuation power was stronger than that of a commercial iodine CT contrast agent (i.e., Ultravistr) at the same atomic concentration and much stronger at the same number density, proving the potential of ultrasmall Yb₂O₃ nanoparticles for use as a powerful CT contrast agent.

Poster Presentation : **PHYS.P-93**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The Counterpoise Correction method used for the basis set superposition effect is failed; where and why?

Nasir Shahzad, Chan Kyung Kim^{1,*}

Department of Chemistry & Chemical Engineering Con, Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

Nowadays, small metal clusters are widely used as catalysts owing to their unique catalytic properties. On the other hand, exploring a suitable bimetallic catalyst for the specific reaction from a pool of homotops is remain a challenging task. To ease this situation, for the initial screening of the catalysts theoretical calculations have been used; for this purpose, adsorption energy (Sabatier's principal) is used as the primary predictor for the catalytic activities. While calculating the intermolecular interactions with finite basis sets we must have to face the basis set superposition effect (BSSE). Owing to BSSE, calculated complexation energies are overestimated; therefore, for accurate measurement of interactions, removal of BSSE is inevitable. Multiple procedures have been designed (using infinite basis set—practically not feasible, chemical Hamiltonian approach—some technical hurdle to apply, self-consistent field for molecular interactions—overcorrect BSSE and counterpoise method) to overcome this problem, a posterior counterpoise correction (CP) method, in this procedure ghost orbitals of partner fragment is used, implemented in different software has been applied extensively. One might expect that CP correction will always weaken the binding interaction, which justifies the variational principle. In contrast, we did not find this trend in all the systems studied here. To unravel the cause of this failure we have performed the systematic study. First, we have confirmed the compatibility of B3PW91 functional with CP method for transition metal clusters because earlier, non-compatibility of some exchange-correlation (XC) functionals were reported. MP2 calculations unravel that this failure is not attributed to the breakdown of XC functionals. Further work explores that, like XC functionals, making basis set empirical may also lead the other theoretical practices meaningless or non-compatible. In this case we have used the basis set LANL2DZ with full effective core potential (ECP), which remove the core electron effect with ansatz value, consequently makes the concept of small perturbation(BSSE) meaningless. Therefore, the empirical basis set results should be used without CP correction.

Poster Presentation : **PHYS.P-94**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Potential Selective H₂S Adsorption onto the Graphene and Doped-Graphene Intervening layers and Reaction with Water to Evolution of Hydrogen and SO₂ as a Function of Reducing Air Pollution

Adhikary Keshab Kumar, Chan Kyung Kim*

Department of Chemistry, Inha University, Korea

To removal of pollutant effectively required judgement accurately to assess the known information, modification and possible alteration in adsorbents such as MOFs, composites and 2D-materials. High performance sorbents and their continuous cope of developments are extremely significant for any gaseous pollutant capture due to its increasing concentration and degradative environmental impact regarding the atmosphere. Here we developed a new possible model based on N-doped graphene's enhanced activity to H₂S adsorption capacity and selectivity. The results showed, the process is selective and specific to the H₂S adsorption. Hence, we can say, the N-doped graphene could be a effective sensor for atmospheric H₂S gas. Use of graphene in the purpose is cost effective but not negligible for the versatile effective nature of graphene. Furthermore, DFT calculations demonstrate the interaction of N-doped graphene pores and H₂S molecules is a contributing phenomenon for an extended level of H₂S uptake and selectivity.

Poster Presentation : **PHYS.P-95**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Conductivity change of ring structure molecules after encapsulation inside single-walled carbon nanotube

Junyoung Lee, Jonghee Yang, Whikun Yi*

Department of Chemistry, Hanyang University, Korea

Single-walled carbon nanotubes (SWNTs) have strong potential for molecular electronics due to their unique structural and electronic properties. We used guest molecules, benzene (C₆H₆), thiophene (C₄H₄S) and benzenethiol (C₆H₅SH). To confirm encapsulation we measured X-ray diffraction (XRD) and Raman spectroscopy. The most obvious difference between pristine and encapsulated SWNT was the reduction or disappeared of peak intensity, which is indexed as (10) reflection and Raman peak position shifted by encapsulation of the guest ring molecules. Such a behavior clearly provides the direct proof of the charge transfer between SWNT and guest molecules with benzene and benzenethiol. The molecular encapsulation of benzene, thiophene and benzenethiol has been analyzed via measuring the conductivity. Currents from measuring I-V curves of encapsulated SWNTs was lower than the pristine SWNTs.

Poster Presentation : **PHYS.P-96**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spectroscopic Demonstration of length-dependent ultrafast depolarization dynamics of a Frenkel exciton in a sterically π -stacked Perylene Bisimide aggregate

Seongsoo Kang, Dongho Kim^{1,*}

Yonsei University, Korea

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Although it is commonly known that π -stacked PBI aggregates of H-type exhibit a red-shifted and broad fluorescence by excimer formation with longer fluorescence lifetimes than monitored for the monomers, unveiling the nascent dynamics of a delocalized Frenkel exciton in molecular π -stacked systems as soon as photoexcitation is still far from being understood. According to our previous time-resolved emission spectroscopic observation of H-type PBI aggregates, it turned out that an initially delocalized Frenkel exciton is localized by ultrafast excimer formation. Furthermore, the migration dynamics of exciton that was not observed in small aggregates having less than four PBI subunits to form one self-assembly was confirmed in only larger aggregates consist of infinite PBI subunits. In terms of rotationally π -stacked displacement of PBI aggregates, the dynamics of a delocalized Frenkel exciton is related to coherent rearrangements of transition dipoles by the interaction between PBI subunits in ultrafast time scale. In this context, we prepared three PBI dyes forming aggregates of three different lengths of the co-facially stacked dimer, tetramer, and extended oligomer in proper conditions. The comparison of depolarization processes according to different sizes of aggregate was performed using polarization-dependent fs-transient absorption anisotropy (TAA) spectroscopic measurements with home-made NOPA pulses of the time duration (50 fs). Since in the ultrafast time window the decay profiles of anisotropy values are not affected by vibrational relaxation and rotational diffusion processes, length-dependent exciton dynamics can reveal fundamental exciton dynamics.

Poster Presentation : **PHYS.P-97**

Physical Chemistry

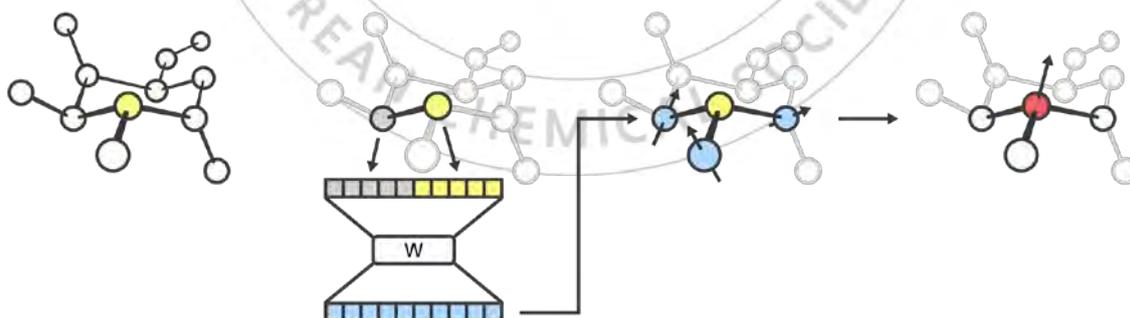
Exhibition Hall 2, FRI 11:00~12:30

Graph Convolutional Neural Network for Understanding Molecular Topology

Hyeoncheol Cho, Insung Choi*

Department of Chemistry, KAIST, Korea

Graph Convolutional Networks (GCNs) have become mainstream of current deep learning approach in chemistry. Enhanced by the ease of generating graph representation of molecules, the target scope of GCNs in the field of chemistry has been expanded from chemical properties to biological activities. Most GCNs that used in current deep learning models ignore three-dimensional structure or rely on the node distances, lacking the spatial structure of molecules. Here, we propose a derivative of GCNs which takes molecular graphs with three-dimensional topology as inputs and recursively updates the scalar and vector features based on the relative positions of nodes. We demonstrate the capabilities of the topological GCN using various tasks among physical, biophysical and physiological prediction tasks.



Poster Presentation : **PHYS.P-98**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A molecular dynamics study of electrolytic systems for EDLC applications

Abdullah Bin faheem, Kyung-koo Lee^{1,*}

Chemistry, Kunsan National University, Pakistan

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

Electric double layer capacitors (EDLC's), also called "super-capacitors" has recently gained traction in the field of energy storage devices because of their high-power density, greater life-cycles, and safety. This study focuses on the properties of the quaternary ammonium salts, 1 dimethylpyrrolidinium tetrafluoroborate, tetraethylammonium tetrafluoroborate, and spiro-1,1'-bipyrrolidinium tetrafluoroborate, dissolved in acetonitrile and propylene carbonate at 1 M concentrations. To explore the properties of the aforementioned systems, an all-atom force field was employed, utilizing the AMBER GAFF force field and quantum mechanical calculations. Molecular Dynamics simulations were performed to study the thermodynamic and transport properties of the said electrolytes. In addition, the microstructure of the simulated systems in terms of radial distribution functions was also examined. In summary, our aim is to provide insight into the difference in their behaviour and aid in the development of future promising materials that can be used in EDLC's.

Poster Presentation : **PHYS.P-99**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Carbon-coated gadolinium oxide nanoparticles for dual-modal imaging

Huan Yue, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this study, we synthesized fluorescence and magnetic resonance dual-modal imaging carbon-coated gadolinium oxide nanoparticles with a good biocompatibility and non-toxic through a facile one-pot process in a solution. The mild synthesis route improves optical properties and the stability of well-defined core-shell structured Gd³⁺ chelated-conjugated carbon nanoparticles. Besides, the carbon-coated gadolinium oxide nanoparticles have a narrow size distribution in the range of 3nm±2nm. In vitro non-toxic confirmed by both DU145 and NCTC1469 cell lines, as well as water proton relaxivity and in vivo MRI of the carbon-coated gadolinium oxide nanoparticles shown a high longitudinal. The products can be used as T1 MRI contrast agent. The optical properties were investigated by Confocal Laser Scanning Microscope at 525nm, the thin carbon layer on the surface of gadolinium oxide nanoparticles showed green color, and under the irradiation of UV light at 365 nm, the carbon nanoparticles showed sky-blue color. As a result, it indicated that the carbon-coated gadolinium oxide nanoparticles can be used as dual mode MR and fluorescence imaging.

Poster Presentation : **PHYS.P-100**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Poly(acrylic acid-co-maleic acid)-coated Gadolinium Oxides Nanoparticles as T₁ MRI contrast agents.

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Paramagnetic Nanoparticles have received great attention in biomedical research because of their physicochemical properties. They have electron spin magnetic moment which improve the quality of magnetic resonance imaging (MRI) preferred technique in diagnosing diseases. Especially, gadolinium oxide (Gd₂O₃) nanoparticles (Gd(III), $s = 7/2$) has one of the largest paramagnetism because 4f-unpaired electrons contribute to magnetic moment. So Gd₂O₃ nanoparticles have been used as promising T₁ MRI contrast agents (T₁ MRI-CAs). In this research, We synthesized Gd₂O₃ nanoparticles coated by the ligands named Poly(acrylic acid-co-maleic acid) (Poly(AA-co-MA)). The colloidal suspension showed great ability as a MRI-CA through relaxivity 1 value. Also, Their biocompatibility was proved by measuring *in vitro* cellular cytotoxicities.

Poster Presentation : **PHYS.P-101**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Intrinsic and Photo-Induced Photoluminescence of Atomically Thin Chromium Thiophosphate (CrPS₄)

Suhyeon Kim, Sunmin Ryu*

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

Ultrathin chromium thiophosphate (CrPS₄) is a promising antiferromagnetic semiconductor with an optical bandgap in the near IR region. In a recent work [1], we proposed that its facile photoreaction is a one-photon photochemical oxidation mediated by photosensitized singlet O₂. In this study, we investigated intrinsic and photo-induced photoluminescence (PL) of CrPS₄ using micro-PL spectroscopy to understand its photophysics and photochemistry. Few-layer CrPS₄ samples were prepared by mechanical exfoliation of bulk crystals and characterized with Raman spectroscopy. The bandgap emission of bulk CrPS₄ appeared at 1.1 eV along with additional emission peaks in the visible region, which was observed similarly for thin CrPS₄ of various thicknesses. In order to reveal which electronic transition is related to the photochemical oxidation, PL and absorption measurements were performed systematically by controlling gas environment and encapsulating sample surfaces with Al₂O₃ films. Temperature dependence and dynamical aspects of the radiative decays will also be discussed. Reference [1] S. Kim, J. Lee, G. Jin, M.-H. Jo, C. Lee and S. Ryu, "Crossover between Photochemical and Photothermal Oxidations of Atomically Thin Magnetic Semiconductor CrPS₄", submitted.

Poster Presentation : **PHYS.P-102**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Detection of Pesticide-like Compounds Using Surface-enhanced Raman Scattering

Eungyeong Park, Sila Jin¹, Yeonju Park¹, Young Mee Jung^{1,*}

Kangwon National University, Korea

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

Many pesticides have been developed to prevent pests and disease. However, excessive use of pesticides has caused to damage with environment and human body. For example, contamination of river and groundwater affects drinking water or residual pesticides may remain in crops. As a result, they are negatively influenced on the respiratory organs, nervous system and caused cancer. Therefore it is important to detect quickly and sensitivity. In our reserch, we tried to detect pesticide-like compounds based on surface-enhanced Raman scattering (SERS). SERS is an ultrasensitive and effective detection method. Details on the result of detection pesticide- like compounds using SERS will be discussed in the presentation.

Poster Presentation : **PHYS.P-103**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Study of characterization and photocatalytic activity of Fe₃O₄@TiO₂- Au magnetic heterostructure

Sila Jin, Chen Lei¹, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

¹*College of Chemistry, Jilin Normal University, China*

Photocatalytic technique is one of the most promising processes for wastewater purification. Among the many semiconductor materials, Fe₃O₄ has the advantage of being magnetically recyclable. Gold nanoparticle also has excellent photocatalytic ability. In this study, we fabricated Fe₃O₄@TiO₂-Au magnetic heterostructure, which can effectively photocatalytic degradate methyl orange (MO) which is a problem of environmental pollution. The properties of Fe₃O₄@TiO₂-Au magnetic heterostructure were investigated by VSM, TEM, XRD, XPS and etc., and the photocatalytic ability was confirmed by UV-Vis and Raman spectroscopy. Details on its characterization and analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-104**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

From the Understanding to the Design of Photochromic Sulfur-Doped Sodalites by a Combined Computational and Experimental Approach.

Antton Curutchet, Mika Lastusaari¹, Eunkyong Kim², Tangui Le Bahers^{3,*}

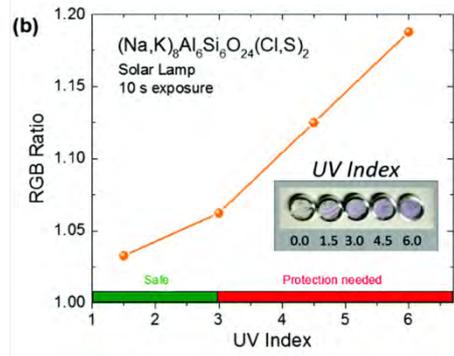
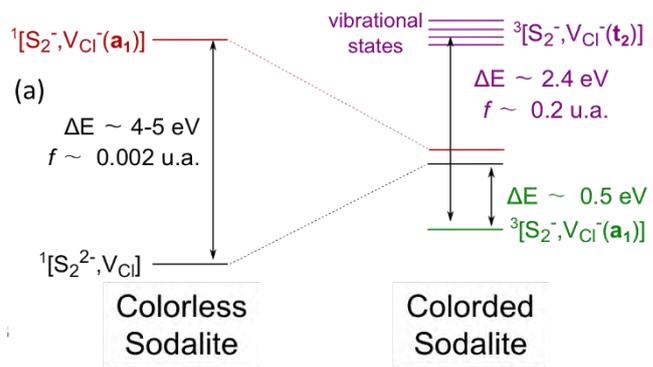
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Photochromic materials are deeply investigated experimentally and theoretically because of their numerous possible high-tech applications going from adaptive glasses to optical memory. Geologists have known for almost one century the existence of natural photochromic minerals of the sodalite family. Although the community is trying to develop new type of photochromic materials, almost no efforts were devoted to understand and develop these photochromic minerals known in geology for a long time. In this presentation, we will start from the natural sulphur-doped sodalite mineral formula to understand its spectroscopic properties. By combining periodic boundary conditions and embedded cluster-type approaches, we bring a theoretical overview of the photochromism mechanism. Our TD-DFT calculations of sodalite systems containing electrons trapped into chlorine vacancies (called F-center) showed absorption spectrum and a simulated color in agreement with experiment. TD-DFT and post-Hartree-Fock calculations were also operated on S_2^{2-} containing systems in order to determine the exact mechanism of coloration and discoloration, supporting that the key step is a direct through space charge-transfer between S_2^{2-} ion and a chlorine vacancy.[1] The bleaching activation energy of 0.3 eV obtained from the quantum chemical calculations is now confirmed experimentally based on a new experimental protocol designed to measure this activation energy [2]. Based on these results, we successfully proposed a way to tune the wavelength of coloration of the artificial sodalites proving that these materials can be easily synthesized and designed for specific applications.[2]References[1] Inorg. Chem. 56, 414 (2017).[2] Mater. Horizons 5, 569 (2018).



Poster Presentation : **PHYS.P-105**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effects of Dielectric Environment on Optical Spectra of Monolayer Tetracene Crystals

Seonghyun Koo, Sunmin Ryu*

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

Wavefunction 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 (Tc) 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 (or hBN) layer was dry-transferred onto Tc film thermally evaporated on a bottom graphene (or hBN) layer. Besides being a confining wall, graphene and hBN also served as an ideal 'spectroscopic window' because of their high optical transparency. Tetracene formed flat films with multiples of its minimum thickness, ~1.2 nm, corresponding to a monolayer and were found stable in the ambient conditions and even under intense laser irradiation. Polarization-resolved photoluminescence (PL) spectra and atomic force microscope (AFM) image showed that Tc films have a long-range order suggesting their crystalline nature. Absorption and PL spectra revealed that there are slight but noticeable energy shifts in major optical transitions between 2D and 3D Tc crystals. PL intensity substantially decreased when supported on graphene compared to on hBN, which indicated efficient energy transfer between Tc and metallic materials. The efficiency of energy transfer was systematically investigated by varying the number of bottom graphene layers. We will also 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-106**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Excited-state proton transfer of 2-naphthol sulfonate derivatives in various water-in-oil microemulsions investigated by fluorescence spectroscopy

Su-Hyun Kang, Han Gook Cho*, Byeong-Seo Cheong*

Department of Chemistry, Incheon National University, Korea

The excited-state proton transfer (ESPT) reactions of several 2-naphthol derivatives having one or two sulfonate groups at different positions were studied in water-in-oil microemulsions formed from various cationic, anionic, and nonionic surfactants. The degree of ESPT reaction in the water pool of microemulsion was estimated by the fluorescence intensity ratio of the two emission bands originated from the protonated and deprotonated forms of 2-naphthol sulfonate photoacids. The different ESPT behaviors were observed depending on the number and position of sulfonate groups in 2-naphthol derivatives as well as the charge of surfactant molecules constituting the reverse micelles. Based on the fluorescence intensity ratios of photoacid dyes in the pool of fixed amount of water ($W_0 = 10$) for each reverse micelle studied, the location and configuration of the dyes in the reverse micelles were suggested, and possible interactions between dyes and surfactants were discussed.

Poster Presentation : **PHYS.P-107**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mechanistic Studies of the 5-Dimethylamino-Naphthalene-1-Sulfonyl Chloride

Han joong Koh

General Science Education, Jeonju National University of Education, Korea

In this study, the solvolysis of 5-dimethylamino-naphthalene-1-sulfonyl chloride was studied by kinetics in binary solvent systems. The rate constants were applied to the extended Grunwald-Winstein equation, using the N_T solvent nucleophilicity scale and Y_{Cl} solvent ionizing scale with sensitivity values of 0.96 and 0.53 for l and m , respectively. These l and m values can be considered to support a S_N2 reaction pathway having similar transition state (TS) structure with that of the benzenesulfonyl chloride reaction. This interpretation is further supported by the activation parameters, i.e., relatively small positive ΔH^\ddagger and large negative ΔS^\ddagger values, and the solvent kinetic isotope effects. Also, the selectivity values obtained in binary solvents were consistent with the proposed mechanism.

Poster Presentation : **PHYS.P-108**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Direct observation of ultrafast symmetry breaking charge separation (SBCS) in perylene bisimide dimer

Yongseok Hong, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

The efficient transport of photon or charge is of critical importance to mimic light-harvesting(LH) systems as well as make photovoltaic devices. In these systems, the de-excitation mechanisms that hinder efficient transport of photon lead to energetically stable sites, which called "trap" state. In turn, the trapping of photons to local sites is a major reason for limited energy transport. Therefore, the understanding how control the trap state plays an important role to enhance the efficiencies of energy transport. Here, we demonstrated that the charge transfer character can restrict the trapping of the photons but activate the ultrafast symmetry breaking charge separation processes. We prepared two kinds of pyridyl substituted PBIs, which are PBI monomer (g2-TIPS) and dimer (g2-CP). The absorption spectra of g2-CP exhibit solvatochromism suggesting the charge transfer (CT) nature of g2-CP. The fluorescence of g2-CP is very weak while the bare PBI dimer shows distinct excimer emission. This difference between bare PBI dimer and g2-CP suggests additional ultrafast decay channel of g2-CP in the excited state such as charge transfer. To obtain further understanding of unique excited state dynamics of g2-CP, we have carried out femtosecond transient absorption measurements in toluene and BCN. Interestingly, the symmetry breaking charge transfer was observed in toluene as well as BCN even though toluene is nonpolar solvent. These results suggest that initially excited state of g2-CP does not form the lowest Frenkel state so-called "trap state" but undergoes efficient charge transfer. In conclusion, we suggest that ultrafast formation of CT exciton facilitates suppression of trapping to local sites.

Poster Presentation : **PHYS.P-109**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characterization of Ultra Small Indium Phosphide Nanoclusters

Juwon Oh, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Recent, colloidal nanocrystalline quantum dots, particularly for Cd-chalcogenide families, have reached a high level of materials. Core/shell QDs that are based on a CdSe quantum dots and a variety of shells are already applied in LEDs for monitors and TV screens. However, there is a strong desire to replace these systems by Cd-free QDs, which should display the same level of performance. In the point that CdSe quantum dots cover visible spectral range, InP quantum dots are considered as one of the most promising heavy-metal-free alternatives. Currently, the optical properties of InP quantum dots are comparable to those of CdSe quantum dots. shells of ZnS, ZnSe, and (Zn,Cd)Se have been developed for InP-based core/shell systems with promising PL quantum efficiencies up to 70%. Moreover, optical absorption and luminescence spectroscopy showed that InP quantum dots have a similar PL peak to their CdSe analogues. However, there is still important problem in an application of InP quantum. Compared to the ease synthetic method for CdSe quantum dots, the preparation of high quality InP quantum dots requires hard delicate efforts due to the rapid precursor conversion process. To solve this difficulty in preparation of high-quality InP quantum dots, magic-sized InP nanocluster has recently been proposed as key conversion intermediates in the synthesis of high-quality InP quantum dots. In this regard, we prepared ultra small InP nanoclusters and characterized their optical and structural properties with their electronic (energy) structures.

Poster Presentation : **PHYS.P-110**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Controllable Optical and Magnetic Properties of Self-doped Mercury Chalcogenide Colloidal Quantum Dots

Danbi Lee, Yun Chang Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

Colloidal quantum dots have been rigorously studied for display, sensor, photovoltaics, and bioimaging. The first steady-state intraband transition of colloidal quantum dots was reported by Jeong et al. in 2014. The steady-state intraband transitions occurring in the conduction band controlled by the electron density can lead the size-dependent absorption and emission in the region of mid-infrared. Therefore, the carrier density is critical to the optical and magnetic properties of the colloidal quantum dots. Here, I present the intrinsic optical and magnetic properties of the colloidal quantum dots determined by the number of electrons in the conduction band by controlling chemical synthesis. Previous studies have focused on the magnetic properties of impurity dopant in the nanocrystal rather than that of nanocrystal itself. The mercury chalcogenide nanocrystals show the mid-IR optical absorption arising from filling electrons into the lowest quantum state by self-doping. The tunable mid-IR intraband absorption at 3-10 μm is correlated with the occupied number of electrons into a discrete electronic state. By monitoring the electron paramagnetic resonance (EPR) spectra, the electron occupation process was thoroughly analyzed, and it turns out that the magnetic property varies from dia-, superpara-, diamagnetic in order during the nanocrystal growth. The singly occupied quantum state (SOQS) with sufficiently long lifetime has a great potential in memory, spintronics, and quantum computing.

Poster Presentation : **PHYS.P-111**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Efficient π - π Stacking of Annulated Rosarin Derivative

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¹*Department of Chemistry, Yonsei University, Korea*

Aromaticity is an important determinant of molecular stability and properties in organic chemistry. Theoretically, molecules with $[4n]$ π -electron systems are known to be unstable, but recently the stable expanded porphyrins with antiaromatic character have been synthesized. Beyond the basic concepts of π -conjugated $[4n]/[4n+2]$ systems, further studies were advanced focusing on the cofacially stacked aromatic/antiaromatic molecules. Parallel fashion of two or more π -conjugated molecules with a short interplanar distance, referred as π - π stacking, determines the basic properties. Stacking of antiaromatic π -systems at close distance is predicted by many previous computational studies that their properties have been weakened or reversed. Through-space interaction allows a delocalization of π -electrons, which reduces their inherent antiaromatic nature in solid or solution state. However, spectroscopic observations to support this suggestion still remain ambiguous so far. Here we propose that the dimeric character of annulated rosarin derivative can be easily controlled by varying the concentration.

Poster Presentation : **PHYS.P-112**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photodissociation of 1-Bromo-3-chlorobenzene

BongGyu Jeong, HyunWook Choi, Jae Kyu Song*, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

Theoretical and experimental branching ratio of ternary cluster cation have been investigated in previous works [1]. The datas of experiments and those of theoretics (Phase Space Theory, PST) were not matched well. Because Rice-Ramsperger-Kassel-Marcus (RRKM) theory predicted well on ternary cluster cation systems, we applied this method to the systems of 1-bromo-3-chlorobenzene (m-BrClBz). The branching ratios of m-BrClBz were obtained by the internal energies of 4.55 and 4.78 eVs. The results of experiments and those of RRKM theory matched well. Binding energies, optimized structures, and frequencies that were necessary elements of RRKM calculations were calculated by Gaussian 09 program set at various theory levels (B3LYP / cc-pVTZ and QZ, wB97X-D / cc-pVTZ and QZ).

Poster Presentation : **PHYS.P-113**

Physical Chemistry

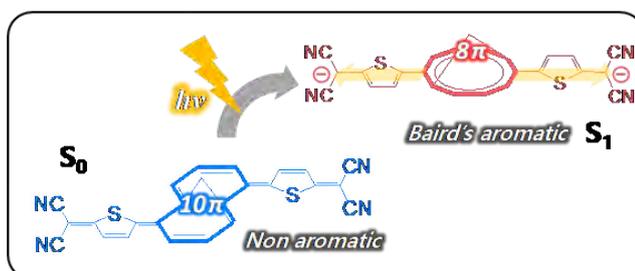
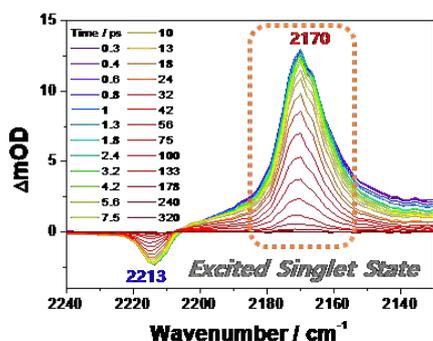
Exhibition Hall 2, FRI 11:00~12:30

Intramolecular Two-Electron Transfer Stabilized by Excited-State Aromatization

Jinseok Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

The excited state aromaticity and its utilization based on Baird's rule have attracted much attention because of its critical role in photochemical reactions. Since structural changes and stabilizations in photosynthesis are dominated by the excited state aromaticity, controlling the excited state aromaticity became essential for designing a new synthetic pathway of photoactive materials. In regarding to this issue, we discovered an intramolecular CT process provokes the aromatization of TMTQ in the excited state. The analysis of C≡N stretching modes by the time-resolved IR spectroscopy revealed that the intramolecular CT process accompanies the shift of electron density towards the dicyano groups (Figure 1). The qualitative analyses of C=C stretching modes and geometry optimization results showed that the CT process leads to a local [8] π formally dicationic M10A core, which becomes aromatic in the excited state by Baird's rule. This observation obviously demonstrates the concept of excited state aromaticity in the annulene system. Furthermore, the CT induced aromatization provides a direct insight into the role of aromaticity in the modulation of excited state properties and designing photoactive materials.



Poster Presentation : **PHYS.P-114**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

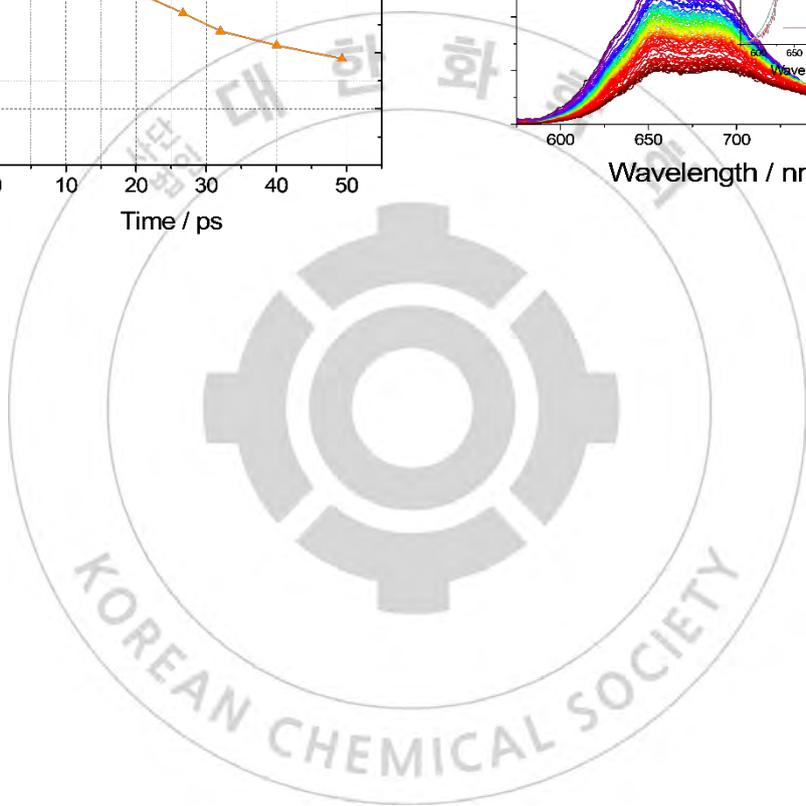
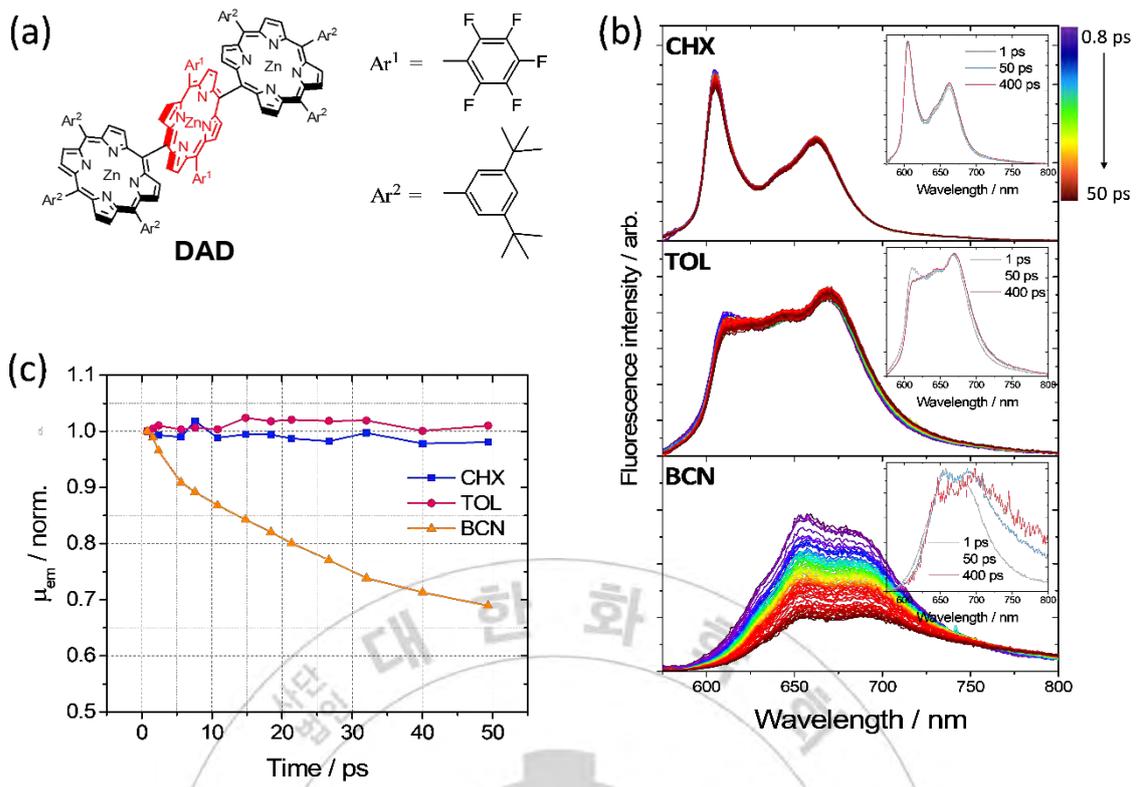
Solvation and Symmetry-Breaking Charge transfer in Porphyrin Triad by Using Broadband Fluorescence Up-conversion Spectroscopy

Taeyeon Kim, Dongho Kim^{1,*}

Department of Chemistry Graduate School, Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

TRF measurements were conducted in three representative solvents (cyclohexane: CHX, toluene: TOL, and benzonitrile: BCN) which can reveal how solvent polarity is related to solvation and SBCT dynamics of DAD in the excited state as shown in Figure 1b. In CHX, TRF spectra is almost unchanged during 50 picoseconds ensuring that exciton is delocalized in the whole molecule as typical porphyrin arrays and this nonpolar solvent does not much affect to (or stabilize) the lowest excited state of DAD. On the contrary, in both TOL and BCN, DAD shows spectral evolution within 50 ps. This observation indicates that solute-solvent interaction effectively contributes to stabilize or change the exciton character. Indeed, the variations in the fluorescence spectra of DAD in TOL, slightly red-shifted and relatively reduced 0-0 vibronic band, was minor compared to those in BCN where the total fluorescence intensity was greatly reduced. We then extracted the emission dipole moments from TRF spectra which can provide evidence of SBCT process as shown in Figure 1c. The emission dipole moment of DAD in BCN was 30% reduced during 50 picoseconds compared to that of Franck-Condon state indicating its reduced orbital overlap between the lowest excited state and the ground state due to SBCT while the emission dipole moments of DAD in CHX and TOL maintained. In conclusion, by using broadband fluorescence up-conversion measurements, we could observe three different cases of solute-solvent interaction in the excited state of DAD depending on solvent polarity: (1) negligible effect (CHX), (2) slight solvation effect on spectral evolution but still maintaining emission transition dipole (TOL), and (3) SBCT process with greatly reduced transition dipole and red-shifted spectra.



Poster Presentation : **PHYS.P-115**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solvent-Modulated Charge-Transfer Resonance in the Excimer State of a Bay-Substituted Perylene Bisimide Dimer

Woojae Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Excimer, which is a linear combination between Frenkel exciton and charge transfer resonance states, is generally regarded as a trap state disrupting desired energy/charge transfer processes in artificial photosynthetic systems. But recently, the excimer has received much attention as a functional intermediate state in the excited-state dynamics such as singlet fission or charge separation processes. In this work, we show that the charge transfer resonance contribution of the excimer state in a bay-substituted perylene bisimide dimer cyclophane can be modulated by dielectric properties of the solvents employed. Solvent-dependent transient fluorescence and absorption measurements show that an enhancement of charge transfer resonance in the excimer state is reflected by incomplete symmetry breaking charge separation processes from the structurally relaxed excimer state with the aid of dipolar solvation processes in the high dielectric environment.

Poster Presentation : **PHYS.P-116**

Physical Chemistry

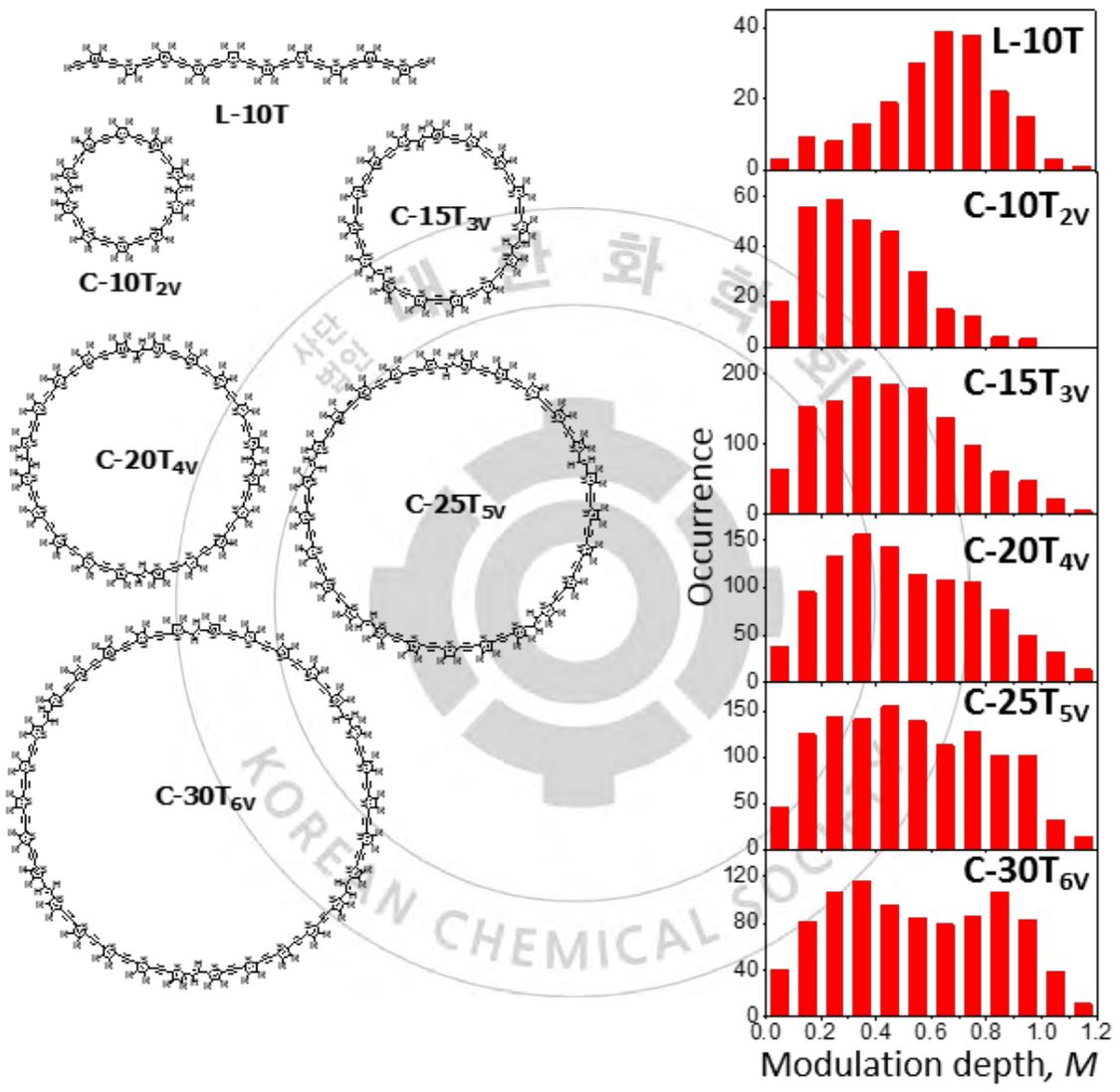
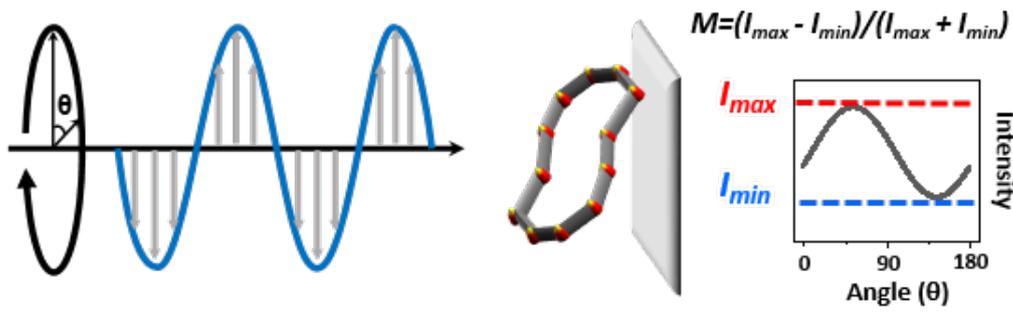
Exhibition Hall 2, FRI 11:00~12:30

Investigation of Conformational Heterogeneity in Large Macrocyclic Thiophenes by Single-Molecule Fluorescence Spectroscopy

Sang Hyeon Lee, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Over the last several decades, there has been substantial interest in conjugated polymers (CPs) for the development of organic optoelectronic devices as light-emitting diodes, light-harvesting apparatus, and transistors. To enhance the performance of CPs in the devices, the planar geometry without torsional defects is needed. This suggests the macrocyclic structure of conjugated oligomers to remove end-effects in linear structures and to lower torsional disorder of carbon backbones [1]. In previous studies, we have studied the molecular size dependence of exciton dynamics [2]. It was concluded that as the ring size increases, the conformational disorder of cyclic systems increases. But these studies on structural information of cyclic oligomers are based on indirect measurement such as vibronic peak ratio with ensemble average. Accordingly, to understand the structural heterogeneity of the large cyclic oligomers, it is required to unveil the conformational structures of cyclic oligomers at the single molecule level. In this regard, we have optically investigated the structures of cyclic oligothiophenes, C-5NT_{NV} (N=2, 3, ..., 6), by using single molecule fluorescence spectroscopy, allowing us to measure the optical properties of single molecules without ensemble averaging. Herein, the conformations of cyclic oligothiophenes depending on the size have been investigated by excitation polarization spectroscopy. The number of excitons in cyclic rings was measured by photon antibunching measurement. References [1] M. Williams-Harry et al. J. Am. Chem. Soc., 130 (2008) 3252-3253. [2] P. Kim et al. J. Phys. Chem. Lett. 6 (2015) 451-456.



Poster Presentation : **PHYS.P-117**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Poly(Acrylic Acid)-RGD Coated Gadolinium Oxides Nanoparticles: Bifunctional Agent for MRI and Gadolinium Neutron Capture Therapy

Son-Long Ho, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

Gadolinium neutron capture therapy (GdNCT) is a cancer-treatment approach that used non-radioactive ^{157}Gd as neutron capture agent. Moreover, ^{157}Gd is also employed as MRI agent to diagnose diseases. Could ^{157}Gd -based compounds be ideally used as theragnostic agents: to track down cancer as MR imaging agent and to treat cancer as GdNCT agent? In this work, gadolinium oxide nanoparticles were coated with poly(acrylic acid)-RGD and were used for theragnostic agents. These NPs showed great MR properties as well as good in vitro and in vivo results as NCT agent against human glioblastoma (U87MG) cell line, due to the presence of linear RGD moiety.

Poster Presentation : **PHYS.P-118**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The role of torsional disorders in exciton self-trapping and delocalization dynamics of [n]cycloparaphenylenes

Jun Oh Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

For the first time, we have comparatively investigated exciton self-trapping and delocalization dynamics in [n]cycloparaphenylenes ([n]CPPs) upon one-photon and two-photon excitations. Exciton delocalization dynamics followed by structural relaxations in the excited states were scrutinized by fs-broadband fluorescence upconversion technique for a series of [n]CPPs. Based on the time-resolved fluorescence spectra, we analyzed changes of 0-1 to 0-0 vibronic peak ratios as a function of time, which reflect the structure and size of excitons in the excited states. Significant differences in the initial values and the changing trends of vibronic peak ratios were observed between one-photon and two-photon excitations. Furthermore, the vibronic peak ratio changes were observed in different temporal regimes suggesting a difference in the rate constants of structural relaxation processes between one-photon and two-photon excitations. We propose that torsional disorders play a significant role in ultrafast exciton self-trapping dynamics and delocalization processes, which accounts for disparate temporal and spectral features upon one- and two-photon excitations. Experimental data are further supported by quantum calculations which exhibit high two-photon absorption cross-section values (GM) for symmetric structures of [n]CPPs with a negligible torsional disorder. Our findings give a solid experimental evidence on conformational heterogeneities of [n]CPPs previously studied by theoretical calculations and provide a further insistence on the role of torsional disorders in conjugation breaks and exciton localizations in the excited-states of pi-conjugated polymers.

Poster Presentation : **PHYS.P-119**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

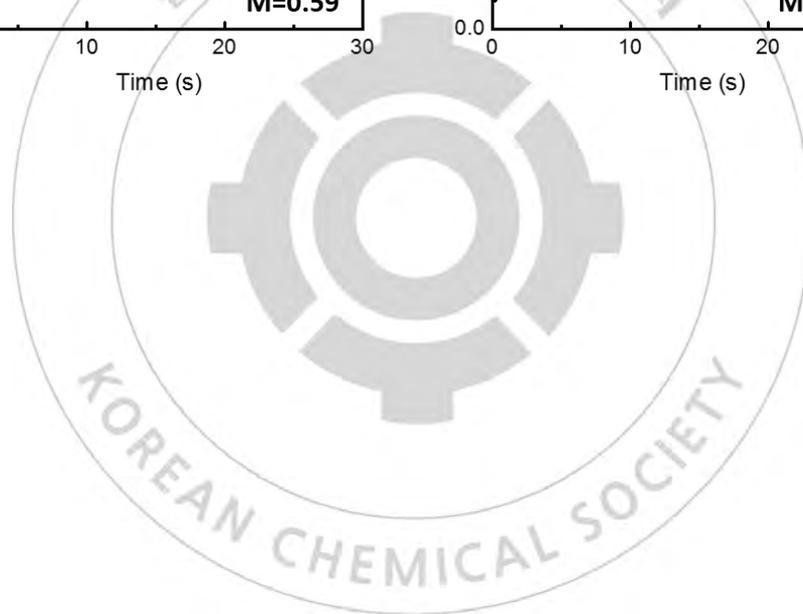
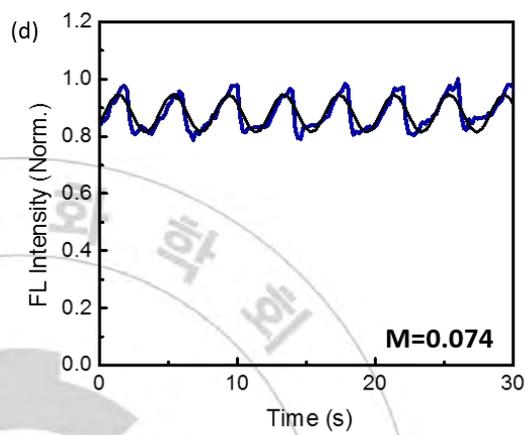
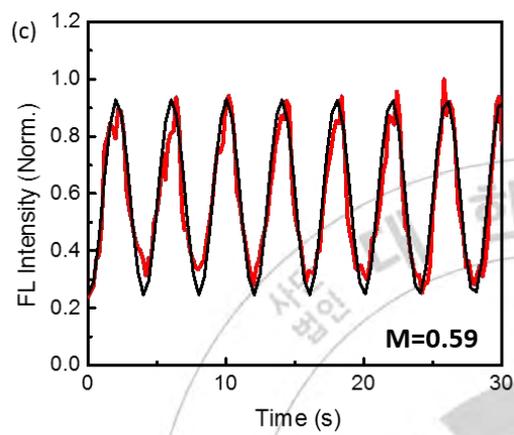
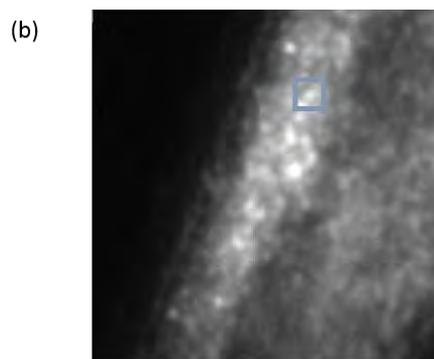
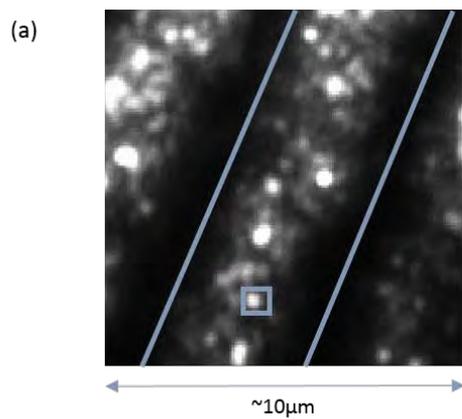
Polarization-Dependent Photoluminescence of Highly (100)-Oriented Perovskite Film

Sangeun Yun, Dongho Kim^{1,*}

Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Lead halide perovskite is an attractive material because of its useful properties, and there have been many studies to figure out its usefulness. The CH₃NH₃PbI₃ thin film which mainly grows in (100) direction was fabricated to clarify the link between the growth pattern and charge carrier dynamics on the perovskite films grown along (100) directions and some spectroscopic studies were performed to understand basic features of the oriented film. Also, we fabricated the perovskite film that grows orthogonal to the glass as a reference. Especially, with 'excitation polarization photoluminescence spectroscopy (ExPPS)' experiment, we could observe an anisotropic absorption of light. Optical absorption is related to the transition dipole moment, and we could conclude that the control of growth direction of perovskite affects the orientation of transition dipole moment by comparing 'modulation depth (M)' value of two different films. Because the optical absorption of the perovskite affects the performance of the perovskite solar cells, we assumed that anisotropic properties of the device of (100) oriented perovskite film that have been reported may have been affected by absorption, and based on other related reports and the growth pattern of the oriented perovskite itself. This study suggests that the anisotropy of the absorption itself can affect the anisotropy in optoelectronic properties.



Poster Presentation : **PHYS.P-120**

Physical Chemistry

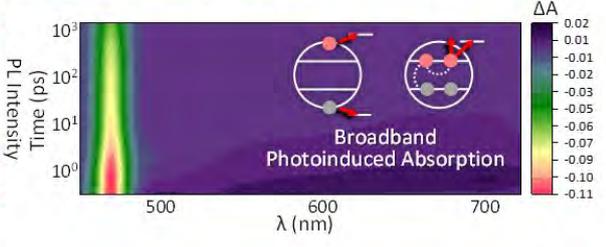
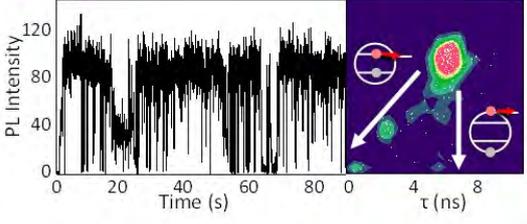
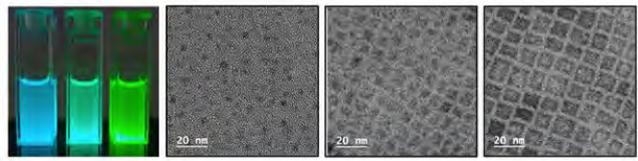
Exhibition Hall 2, FRI 11:00~12:30

Elucidation of Photoluminescence Blinking Mechanism and Multiexciton Dynamics in Hybrid Organic-Inorganic Perovskite Quantum Dots

Taehee Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Halide perovskites (ABX_3) have emerged as promising materials in the past decade owing to their superior photophysical properties. In order to optimize their utilization into optoelectronic devices, fundamental understanding of the optical behaviors is necessary. In order to reveal the comprehensive structure-property relationship, $CH_3NH_3PbBr_3$ (**MAPbBr₃**) perovskite quantum dots of three different sizes were prepared by controlling the precipitation temperature. Photoluminescence (PL) blinking, a key process that governs the emission efficiency of the PQD materials, was investigated in detail by the time-resolved spectroscopic measurements of individual dots. The photophysical description of the underlying mechanism of PL blinking processes was provided through the dot-to-dot analysis of lifetime-intensity scaling. The nature of the generated species in the course of blinking events was identified, and the mechanism governing the PL blinking was studied as a function of PQD sizes. Further, the practical applicability of **MAPbBr₃** PQDs was assessed by studying the multiexciton dynamics under high photoexcitation intensity under which most of the display devices work. Ultrafast transient absorption spectroscopy helped uncovering the volume-dependent Auger recombination rates from which the potential role of organic cation was suggested in suppressing Auger recombination at small PQD volume regime. The size-dependent trend in Auger recombination was further explored by comparing the early-time transitions related to surface trap states and higher band states.



Poster Presentation : **PHYS.P-121**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Aqueous Bimolecular Proton Transfer in Acid-base Reaction using Femtosecond Infrared Spectroscopy

CheongHa Lim, JuHyang Shin, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Femtosecond infrared spectroscopy was used to observe aqueous bimolecular proton transfer as well as general acid-base reaction after photoexcitation of 8-hydroxypyrene-1,3,6-trisulfonic acid (HPTS), a photoacid that can become a strong acid when electronically excited. Excited HPTS became a strong acid with $pK_a = 0.0$ from $pK_a = 6.6$ in the ground state. Azide (N_3^-), which has a strong band at 2042 cm^{-1} and its conjugated acid (DN_3) at 2133 cm^{-1} , was used as a base. When the mixture of HPTS and N_3^- in D_2O solution was excited at 400 nm in the low base concentration ($< 150\text{ mM } N_3^-$), the dominant reaction path was found to be the bimolecular reaction between the base molecule and deuteron (D^+) which was dissociated from HPTS in the excited state ($HPTS^*$), rather than direct reaction resulted from acid-base complexes that was observed in high base concentration. HPTS became $HPTS^*$ on the subpicosecond timescale, which release one D^+ leaving $HPTS^*$. The $HPTS^*$ returns to the ground state, $HPTS^-$ before it rebinds D^+ to become HPTS. Four species HPTS, $HPTS^*$, $HPTS^-$, and $HPTS^-$ were identified by their characteristic vibrational band in the region of $1400\text{--}1670\text{ cm}^{-1}$ and their kinetics were determined. Kinetics of N_3^- and DN_3 , determined by their absorption bands in 2042 and 2133 cm^{-1} , respectively, were found to be the same. The bimolecular reaction involved in acid-base reaction observed via this research will be presented.

Poster Presentation : **PHYS.P-122**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Branching ratio about ternary cluster cations

HyunWook Choi, Jae Kyu Song*, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

In our previous study, we measured the branching ratios about dissociation of two solvent molecules in six ternary cluster cations, aniline-water-ethanol cation (AWE⁺), aniline-water-isopropanol cation (AWP⁺), aniline-methanol-ethanol cation (AME⁺), aniline-water-methanol cation (AWM⁺), aniline-water-pyrrole cation (AWPy⁺), and aniline-water-benzene cation (AWB⁺). We tried to explain the branching ratios theoretically using the phase space theory (PST) because the dissociation of solvent molecules occurred through loose transition states (TS) which did not have any barriers of reverse reaction. In the PST, an orbiting transition state (OTS) located at the maximum of the long range effective potential was assumed and the rotational constant and vibrational frequencies of the products were used in the rate constant calculations. However, the OTS/PST calculations could not explain the experimental branching ratios. Although it was hard to apply the conventional Rice-Ramsperger-Kassel-Marcus (RRKM) theory on ternary cluster cation because of loose TS, we could predict the experimental result with RRKM theory applying simple assumption.

Poster Presentation : **PHYS.P-123**

Physical Chemistry

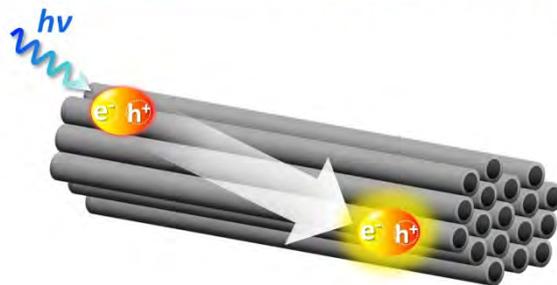
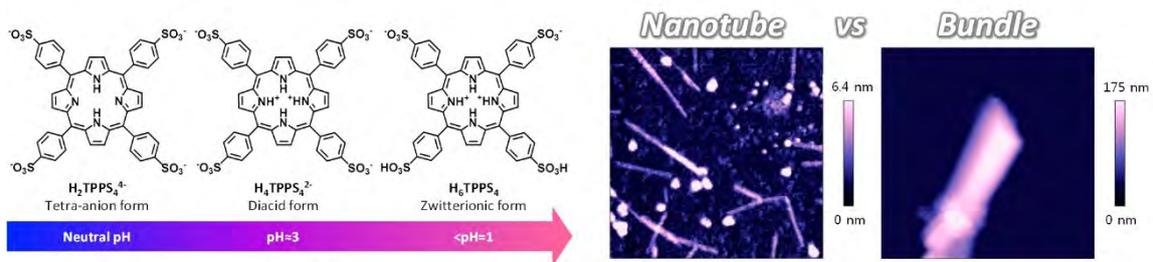
Exhibition Hall 2, FRI 11:00~12:30

Enhancement of Exciton Transport in Porphyrin Aggregate Nanostructures by Controlling the Hierarchical Self-Assembly

Taehee Kim, Sang Hyeon Lee, Yongseok Hong, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Exciton transport in meso-tetra(4-sulfonatophenyl) porphyrin (TPPS) J-aggregates was directly imaged using the emission profile analysis method with confocal fluorescence microscopy. By controlling the structural hierarchy of TPPS aggregates, we could comparatively study the exciton transport properties in single nanotubes and bundled structures. Using the one-dimensional diffusion model, the exciton diffusion coefficients of TPPS nanotubes and bundles were estimated as 95 and 393 nm² ps⁻¹, respectively, showing a dramatic enhancement of exciton transport in bundled structures. To reveal the underlying mechanism of enhanced exciton transport in bundle compared to that in single strands, the spatially resolved measurements of exciton transport images were correlated with the spectral information at each local sites. We have confirmed that nanotube and its bundled form possess different energetic landscapes and exciton migration dynamics. Agglomeration into bundles led to an increase in system-environment coupling and denser distribution of energy states, facilitating longer migration length and accelerated transport. Detailed analysis in this study provides important insights into the structure-dependent exciton transport properties of self-assembled J-aggregate nanostructures.



Poster Presentation : **PHYS.P-124**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A conformational study of 4-bromo-1-butene using chirped-pulse Fourier-transform microwave spectroscopy

Heesu Jang, Rebecca A. Peebles¹, Sean A. Peebles¹, Jung Jin Oh*

Department of Chemistry, Sookmyung Women's University, Korea

¹*Department of Chemistry and Biochemistry, Eastern Illinois University, United States*

The rotational spectrum of 4-bromo-1-butene ($\text{BrCH}_2\text{CH}_2\text{CH}=\text{CH}_2$) has been recorded in the range 2-9 GHz using a chirped-pulse Fourier-transform microwave spectrometer. For all five possible conformations—*ga*, *gg*, *gg'*, *sa*, and *sg*, *ab initio* optimization and energy calculations were performed. The *ga* conformer has the lowest energy, and for this conformer, 81 hyperfine components were assigned from $J = 2$ to $J = 7$ for both ^{79}Br and ^{81}Br isotopologues, respectively. Only 44 hyperfine components were assigned for two isotopologues of the *gg* conformers, respectively. The rotational constants, centrifugal distortion constants, and nuclear quadrupole coupling constants were determined for two isotopologues of the *ga* and *gg* conformers, respectively. The experimental results were compared with the *ab initio* calculated values."This work is financially supported by Korea Ministry of Environment(MOE) as 「Graduate School specialized in Climate Change」."

Poster Presentation : **PHYS.P-125**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photodissociation Dynamics of CF₂I₂ in Solution Probed by Time-Resolved Infrared Spectroscopy

Seongchul Park, JuHyang Shin, Hojeong Yoon, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Photodissociation dynamics of CF₂I₂ dissolved in *c*-C₆H₁₂ was investigated by time-resolved infrared spectroscopy. 267-nm excitation leads to exclusive three-body decay and 350-nm to exclusive two-body decay. As a result of these exclusive decay, some reaction intermediates (CF₂, CF₂I, I-CF₂, iso-CF₂I₂) and product (C₂F₄) were detected. Each chemical species shows characteristic C-F stretching frequencies: 1097 cm⁻¹ for CF₂, 1166 and 1118 cm⁻¹ for CF₂I, 1072 cm⁻¹ for CF₂ interacting with departing I atom, 1157 cm⁻¹ for an isomer of the reactant and 1176 cm⁻¹ for product C₂F₄. These frequencies were confirmed by Ar matrix experiment and DFT calculations.¹ When excited at 267 nm, dissociated I atoms from 33% of a reacting molecule escape the solvent cage efficiently. CF₂I (38%) 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 the remaining CF₂ (62%) bimolecularly binds to produce C₂F₄ with a diffusion-limited rate. When excited at 350 nm, CF₂ is produced via I₂-CF₂ isomer with a time constant of 14 ps that is rapidly formed from CF₂I and the dissociated I atom with a time constant of 0.5 ps. About 51% of CF₂I radical does not form the isomer and geminately rebinds with I atom with time constants of 140 ps (15%) and 36 ns (34%). The photo-produced CF₂I appears to interact with solvent in three different ways; one leads to isomer formation, the others lead to fast and slow GRs. 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-126**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Rebinding Dynamics of CO with Cytoglobin in Aqueous Solution Investigated by Time-resolved Vibrational Spectroscopy

JuHyang Shin, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Time-resolved vibrational spectroscopy was used to prove the rebinding dynamics of CO to cytoglobin (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 2.5 ns decay but the A₁ and A₃ bands decay with a time constant of 280 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 modeled 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-127**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Dynamics of NO release from Photoexcited Roussin`s Red Ester Probed by Time-resolved Infrared Spectroscopy

Hojeong Yoon, Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Nitric Oxide (NO) plays various important physiological roles in vivo. Roussin`s red ester (RRE), one of the nitrosyl-clusters of iron and sulfur that is stable and less toxic and releases NO by UV-light, can a good NO-donor. We have studied the dynamics of the RRE's photochemistry in D₂O using femtosecond infrared (IR) spectroscopy. RRE has a large IR absorption in the NO stretching mode in the spectral region of 1850~1650 cm⁻¹. Time-resolved IR spectra were measured in the NO stretching region after excitation with various wavelengths (310, 360, and 400 nm). With the help of (TD)DFT calculations, transient absorptions were attributed to a meta-stable RRE (MS) and RRE radical that released one NO from RRE. Fraction (40~60%) of excited RRE undergoes photodeligation releasing one NO and the remaining molecules relaxes to the ground state via the MS. Some of the produced RRE radical geminately recombines with NO, resulting in only fraction (18 ~ 45%) of the excited RRE produces NO that remains in solution before it can participate in the biological function. The primary quantum yield (QY) for NO deligation as well as the yield for the geminate recombination (GR) depend on the excitation wavelength. It appears that GR yield decreases as the excitation energy increases, suggesting that the produced NO has a higher kinetic energy that separates NO faster from the RRE radical. However, the QY does not show gradual dependency on the excitation energy, suggesting that many excitation states are reached by a UV excitation. The optimal excitation wavelength for most usable NO release will be discussed.

Poster Presentation : **PHYS.P-128**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Femtosecond pump-probe experiments at hard X-ray scattering & spectroscopy (XSS) beamline, PAL-XFEL

Jae Hyuk Lee

PAL-XFEL, Pohang Accelerator Laboratory, Korea

The hard X-ray scattering & spectroscopy (XSS) beamline at PAL-XFEL (Pohang Accelerator Laboratory's X-ray Free Electron Laser) has started the user service since June 2017. PAL-XFEL has three beamlines, two for hard X-ray and one for soft X-ray. XSS is the one of the hard X-ray beamlines dedicated to time-resolved X-ray experiment. X-rays from PAL-XFEL are ultra-bright ($\sim 5 \times 10^{11}$ photons/pulse at 9.7 keV) and ultra-short (



Poster Presentation : **PHYS.P-129**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Analysis on anisotropic effects of diffusion-influenced reactions

Dajeong Choi, Hyojoon Kim*, Taejun Kim*

Department of Chemistry, Dong-A University, Korea

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-130**

Physical Chemistry

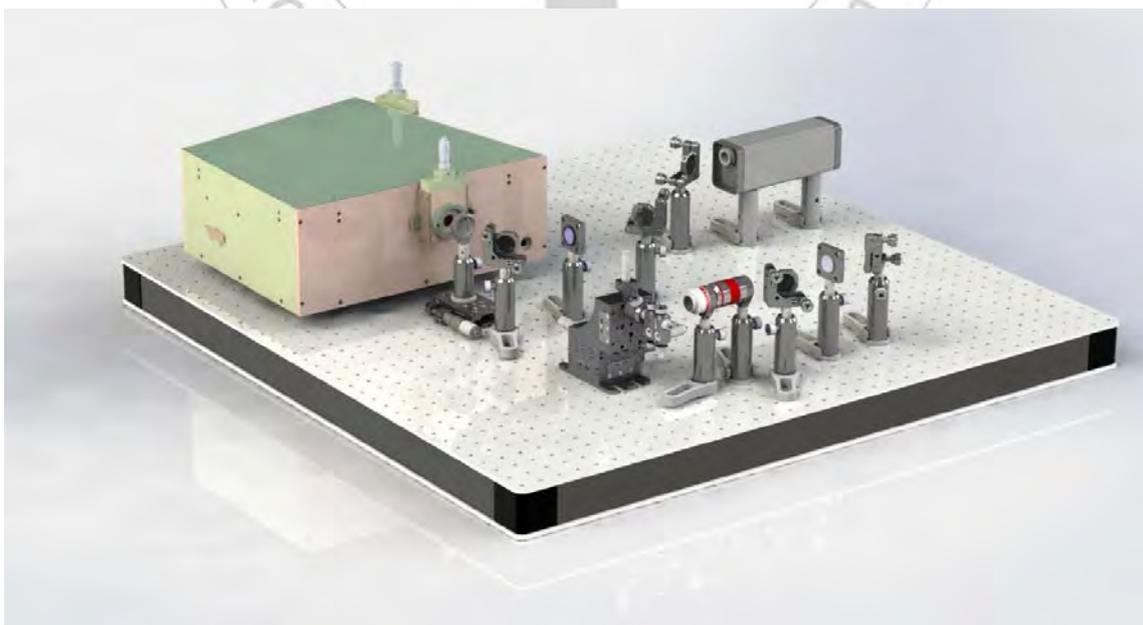
Exhibition Hall 2, FRI 11:00~12:30

Development of versatile spectrometer for ultralow-frequency (50 cm^{-1}) Raman and Photo Luminescence measurement of MAPBI₃ Perovskite.

Mingyeong Shin, Juwon Kim, Myeongkee Park*

Department of Chemistry, Dong-A University, Korea

We have developed a Raman spectrometer for ultralow-frequency (50 cm^{-1}) Raman and Photo luminescence measurements of MAPBI₃ Perovskite, which is critical to know how MAPBI₃ Perovskite is distorted after getting excited. The experimental Raman setup consists of a 488.05 nm laser, 488 nm transmission filter, 3x beam expander, 25x objective lens and notch filter. We measured the M2 to determine the laser beam quality. The M2 is found to be 1.32 by using the knife-edge method. The focused spot area is $\sim 7 \text{ mm}^2$. In addition we have developed Raman cross-sections of MAPBI₃ by comparing cyclohexane Raman.



Poster Presentation : **PHYS.P-131**

Physical Chemistry

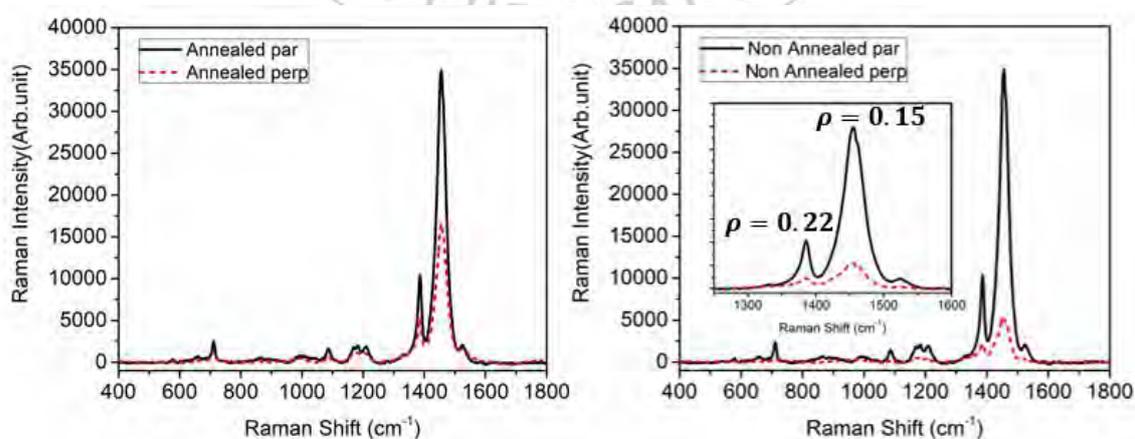
Exhibition Hall 2, FRI 11:00~12:30

Structural Dependence on Intermolecular π - π Interaction of Poly(3-hexylthiophene) Probed by Polarized Raman Spectroscopy and Theoretical Calculation

Juwon Kim, Mingyeong Shin, Myeongkee Park*

Department of Chemistry, Dong-A University, Korea

A conductive polymer, poly(3-hexylthiophene) (P3HT) has been widely used for photovoltaic applications. Highly π -conjugated poly(3-hexyl-thiophene) has effective intermolecular π - π overlaps which provide high charge-carrier performance for photovoltaics. To elucidate its structural dependence on the intermolecular interactions, we have studied vibrational Raman modes and depolarization ratios of annealed and non-annealed P3HT films. It is found that the annealed film shows greater depolarization ratios of 0.34 in compared to 0.15 of the non-annealed film indicating that the annealed one has stronger π - π conjugation overlaps. This result is supported by that parallel-stacked thiophene which exhibits greater depolarization ratio of 0.45 than 0.37 of twisted-stacked structure by MP2 theory. We demonstrate polarized Raman spectroscopy can be employed in assessing the molecular alignments.



Poster Presentation : **PHYS.P-132**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Increased reaction rate by near-degenerate multiple reaction pathways in oxidative addition of chlorobenzene to POP rhodium complex

Hyo Weon Jang

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Recently, a quantum simulation of reaction pathway for the title-mentioned organometallic reaction was reported with a calculation of activation Gibbs energy about 35kcal/mol, which is supposed to be compared to the experimental findings of 24 hours of reaction time at room temperature. Our observation that the calculated energy seems to be too high to account for the experimental results leads us to search for additional reaction pathways connecting the reactant via multiple transition states with nearly degenerate activation Gibbs energies to identical oxidatively added product of chlorobenzene to POP rhodium complex with success. With the additional pathways, the agreement between simulation and experiment improves.



Poster Presentation : **PHYS.P-133**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Excited state hydroxide ion dissociation reaction of an Arrhenius photobase

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Department of Chemistry, Korea University, Korea

Arrhenius photobases are organic bases of which the pK_b is significantly decreased following electronic excitation and hydroxide ion is dissociated. A photobase with acridine moiety (Acr-OH) is designed and synthesized to study excited state hydroxide ion dissociation reactions in polar solvents. The pK_b value of Acr-OH is estimated by using density functional theory calculations and is found to be in excellent agreement with the experimentally determined pK_b value. Thermodynamic properties of Acr-OH in aqueous solutions are studied by using temperature-dependent UV-visible absorption spectroscopy. The photophysical properties of Acr-OH in polar solvents are studied by using UV-visible absorption, steady-state fluorescence, and time-resolved fluorescence spectroscopy. The excited state hydroxide ion dissociation reactions in polar solvents will be presented.

Poster Presentation : **PHYS.P-134**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Headgroup Effect on the Formation of Self-Assembled Monolayers on Au(111) by Adsorption of 2-Phenylethyl Thiocyanate and 2-Phenylethyl Selenocyanate

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Self-assembled monolayers (SAMs) of aromatic thiol have received great interest because of their electrical and optical properties that offer attractive applications in molecular switching, molecular electronics, and electronic interfaces. Aromatic SAMs with various headgroup or methylene spacer are studied to acquire highly ordered aromatic SAMs. In this study, we investigated the headgroup effect on the formation of 2-phenylethyl thiocyanate (2-PET) and 2-phenylethyl selenocyanate (2-PES) SAMs on Au(111) from ambient-pressure vapor deposition by scanning tunneling microscopy (STM) and cyclic voltammetry (CV). STM observation showed that the surface structure both 2-PET and 2-PES SAMs were strongly influenced by deposition temperature and time. The 2-PES SAMs on Au(111) at 363 K for 6 h have a ($\sqrt{3} \times \sqrt{3}$) structure with long-range ordered phase, whereas 2-PET SAMs have mixed phase with ordered and disordered domains. In addition, CV measurements showed that reductive desorption potential for 2-PES SAMs at -940 mV was higher than that for 2-PET SAMs at -887 mV, which means that the Se-Au interaction for 2-PES SAMs is stronger than the S-Au interaction for 2-PET SAMs.

Poster Presentation : **PHYS.P-135**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Surface Morphology and Reductive Desorption Behavior of Self-Assembled Monolayers on Au(111) Derived from Aromatic Dithiol and Diselenol

Young Ji Son, Jaegun Noh*

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Self-assembled monolayers (SAMs) containing aromatic thiol and selenol have been widely used for various applications in molecular electronics, corrosion inhibition, and bio-interfaces due to their chemical stability and functional manipulation. To understand the surface structures and binding conditions of SAMs depending on the number of phenyl ring and the type of headgroup, we examine the structural properties and reductive desorption behavior of dithiol- and diselenol-based self-assembled monolayers formed from benzenedithiol (BDT), biphenyldithiol (BPDT), and benzenediselenol (BDSe) using scanning tunneling microscopy (STM) and cyclic voltammetry (CV). STM measurements showed that both BDT SAMs formed from a 1 mM ethanolic solution and BDSe SAMs formed from 10 μ M DMF solution have striped phase in which molecular backbone are oriented parallel to the gold surface. In addition, reductive peak of BPDT SAMs was observed at more negative potential of -869 mV compared to thiol-based BDT SAMs (-773 mV) because of longer phenyl chain. Also, desorption peak of BDSe was appeared at -830 mV, suggesting that Se-Au bonding is stronger than S-Au bonding.

Poster Presentation : **PHYS.P-136**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Formation and Growth of Pentafluoroselenolate Self-assembled Monolayers on Au(111) at High Temperature

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Self-assembled monolayers (SAMs) are simple and versatile method to modify solid surfaces. Recently, there have been a lot of researches studying SAMs formed from fluorinated aromatic molecules, because of their excellent electrical conductivity and prospect for applications on electronic devices. From previous papers, it was reported that the structural properties of the SAMs are key factor in modification of the surface energy level. In this regard, we investigated molecular structure of pentafluorobenzeneselenolate (PFBSe) SAMs. The SAM samples were deposited at high temperature to obtain high quality SAMs. The prepared samples were characterized by scanning tunneling microscopy (STM) and cyclic voltammetry using reductive desorption method (RD) to elucidate structure and electrochemical behavior of the SAMs. The PFBSe SAMs showed highly ordered structures with many adatom islands at early stage of deposition. As the deposition time increases, the number of adatom islands decreased and wider terraces appeared. High-resolution STM observations revealed that PFBSe SAMs form $(14 \times \sqrt{3})$ lattice structure after deposition of 5 min and form $(5\sqrt{3} \times \sqrt{3})$ lattice structure after deposition of 30 min. RD results showed that the PFBSe SAMs formed at 373 K for 30 min to 1 h were more stable than the others.

Poster Presentation : **PHYS.P-137**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photoionization of cyclopentanone conformers and photodissociation of the corresponding cation using high resolution vacuum ultraviolet mass analyzed threshold ionization (VUV-MATI) spectroscopy

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New and Renewable Energy Research Center, Ewha Womans University, Korea

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Cyclopentanone, which is a versatile synthetic intermediate, being a precursor to drugs or fragrances, has a ring-puckering vibration of the out-of-plan C=O bond. Since the ring-puckering vibration has the double-well potential with the barrier height of 680 cm^{-1} in the neutral state, it is known that the interconversion between the twist and the envelop conformers occurs along the pseudorotational coordinate associated with twist and bending motions, where the barrier height is lower than that of the ring-puckering coordinate. To identify the conformational structures and determine the adiabatic ionization energy (AIE) of corresponding conformer, the high-resolution vibrational spectrum of cyclopentanone cation has been recorded by employing the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) technique. From the measured MATI spectrum, the accurate ionization energy of cyclopentanone was determined to be $74,771 \pm 3\text{ cm}^{-1}$ ($9.2704 \pm 0.0004\text{ eV}$) under the zero field limit, which would correspond to AIE of the twist conformer based on the quantum chemical calculations. Vibrational assignments of the peaks observed in the MATI spectrum could be achieved utilizing the Franck-Condon simulations at the B3LYP/cc-pVTZ level. In addition, we measured the appearance energy for $\text{C}_5\text{H}_8\text{O} \rightarrow \text{C}_4\text{H}_8^+ + \text{CO} + \text{e}^-$, being 9.7053 eV , which is lower than the previous value of 9.86 eV by multiphoton ionization and dissociation study. We will present the theoretical results on photodissociation dynamics of the corresponding cation in cyclopentanone conformers.

Poster Presentation : **PHYS.P-138**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhancement the photovoltaic performance of perovskite solar cells with improvement on down converting properties of Eu-PDMS complex detachable film

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¹*Institute of Basic Science, Sungkyunkwan University, Korea*

Recently, on the basis of many advantages, perovskite solar cells have exhibited outstanding character for photoelectric conversion and one certified power conversion efficiency 22.1%. $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cells have high power conversion efficiency but poor stability of ultraviolet irradiation. Therefore, it is necessary to study for prevention of degradation perovskite solar cells for ultraviolet light. In this research, we are synthesized Eu-bathophenanthroline complex powder for visible light conversion to ultraviolet. Also, we were developed the transparent Eu-PDMS complex detachable films via controlling the Eu powder. As a result, an about 20% improvement in conversion efficiency was achieved after introducing the 100 ul-Eu-PDMS complex film, which also surpassed the reference device, which mainly results from increasing light harvesting efficiency by down conversion effect.

Poster Presentation : **PHYS.P-139**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Conformational preference and cationic structure of 2-methylpyrazine by VUV-MATI spectroscopy and natural bond orbital analysis

Do Won Kang, Hong Lae Kim, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

Alkylpyrazines well known as aromatic substances or traditional medicines are the interesting molecular systems with the methyl conformations based on pyrazine concerned to unique structural and dynamical properties. We explored the conformational preference by the methyl group and the highest occupied molecular orbitals (HOMOs) of 2-methylpyrazine and its cation as a precursor of alkylpyrazines utilizing the high-resolution one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy and the natural bond orbital (NBO) analysis, in order to understand the relevant molecular activities. The measured VUV-MATI spectrum of 2-methylpyrazine reveals the adiabatic ionization energy of the molecule and the vibrational frequencies of the corresponding cation. From the 0-0 band position in the MATI spectrum under the zero-field limit, the accurate adiabatic ionization energy was determined as 9.0439 ± 0.0006 eV ($72,944 \pm 5$ cm⁻¹), which is lower than that of pyrazine. The peaks observed in the spectrum could unambiguously be assigned on the basis of the vibrational frequencies and the Franck-Condon factors for the individual totally symmetric transitions between the S₀ and the D₀ states according to the simple one-photon dipole selection rules. From the spectral simulation called the Franck-Condon fit, the most convincing molecular structure of the 2-methylpyrazine cation has been determined. Upon ionization by removal of an electron from the non-bonding orbital (HOMO) on the para nitrogen atoms, a significant structural change takes place along the vibrational motion, ν_{20} associated with ring distortion by contraction of NN distance, resulting in prominent its overtones and combination bands with other vibrational modes in the spectrum. It reveals that the methyl substitution in pyrazine lowered the adiabatic ionization energy, where the methyl group against the pyrazine moiety preferred the anti-configuration on the D₀ state, resulting in the frozen internal rotation regardless of ionization process.

Poster Presentation : **PHYS.P-140**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Conformational structure of cationic tetrahydropyran by VUV-MATI spectroscopy

So Young Eom, Do Won Kang, Hong Lae Kim, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

Tetrahydropyran (THP) as a saturated six-membered heterocyclic compound possessing an oxygen atom has been paid much attention and still considered in a regard of ionization dynamics related to HOMO and ring-puckering potentials depending on heteroatom such as O. In order to investigate the conformational structures affected by ionization, we measured the vibrational spectrum of THP cation in the ground electronic state using the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) technique. Successfully, accurate ionization energy of THP based on the measured VUV-PIE curve and the origin band of VUV-MATI spectrum was determined to be $74,687 \pm 3 \text{ cm}^{-1}$ ($9.2600 \pm 0.0004 \text{ eV}$). The measured VUV-MATI spectra could be analyzed by the Franck-Condon simulations obtained with the optimized structures and the vibrational frequencies for the S_0 and the D_0 states calculated at the density functional theory level, which reveals the stable conformation structure for THP.

Poster Presentation : **PHYS.P-141**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photoionization study of non-volatile molecules in the gas-phase by IR desorption/VUV single photoionization spectroscopy

Sung Man Park, Jaehwan Choi, Hong Lae Kim, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

Mass spectrometry through thermal vaporization can be applicable to non-volatile or biological molecules, but it is not suitable method because of thermal decomposition of the molecules. In order to generate non-volatile molecules in the gas-phase and ionize them, we have developed the IR laser desorption and VUV laser ionization mass spectrometry using carbon powder as a matrix in the MALDI. Therein, non-volatile molecules are introduced to photoionization chamber picking-up by supersonic jet of carrier gas such as He or Ar after desorption by infrared laser. Then, the desorbed molecule introduced into the PI chamber can be ionized by VUV single photon ionization. We have measured the photoionization efficiency curves of some non-volatile organic molecules, from which their adiabatic ionization energies were determined.

Poster Presentation : **PHYS.P-142**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

High resolution vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of 2-chloropyridine: Determination of adiabatic ionization energy and cationic structure

Nayoung Choi, Yu Ran Lee¹, Hong Lae Kim, Chan Ho Kwon*

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¹*New and Renewable Energy Research Center, Ewha Womans University, Korea*

Pyridine substituted by a nitrogen atom in benzene has been known as a unit molecule of bioactive compounds as well as a precursor displaying the complicated photophysical process in the excited state. In this respect, much attention has been paid to the molecular structure and the highest occupied molecular orbital (HOMO) affected by substitution of the halogen atom in pyridine such as 2-chloropyridine (2CP). We measured the vibrational spectrum of cationic 2CP by the one-photon mass-analyzed threshold ionization (MATI) spectroscopy using vacuum ultraviolet (VUV) pulse generated by four wave mixing in the Kr cell. The MATI spectrum of 2CP displays the most intense 0-0 band unlike pyridine cation, which indicates little geometrical change upon ionization. Based on the vacuum ultraviolet photoionization efficiency curve of 2CP, the accurate adiabatic ionization energy of 2CP was determined to be 9.4743 ± 0.0004 eV ($76,415 \pm 3$ cm⁻¹) under the zero-field limit of the 0-0 band in the MATI spectrum, which is very different with the previous value of 9.63 eV by photoelectron spectroscopy. Most of the peaks observed in the VUV-MATI spectra could be assigned by utilizing the Franck-Condon factors and vibrational frequencies calculated through adjustments of the geometrical parameters of cationic 2CP at the ω B97XD/aug-cc-pVTZ level.

Poster Presentation : **PHYS.P-143**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

One-photon Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy (VUV-MATI) of methyl vinyl ketone : Determination of Composition of *s-trans* and *s-cis* conformers

Jaehwan Choi, Sung Man Park, Hong Lae Kim, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

Methyl vinyl ketone (MVK) which is an α,β -unsaturated ketone has two conformations of *s-trans* and *s-cis*, which can be interconverted by rotation of the single bond between the C=C bond and the C=O bond. It was reported that the composition at room temperature was 7 : 3 for *s-trans* and *s-cis* conformers. We measured the identifiable vibrational spectra of the cationic MVK conformers using one-photon mass-analyzed threshold ionization (MATI) spectroscopy with the vacuum ultraviolet (VUV) radiation generated by four-wave difference frequency mixing in Kr gas. From the origin band in the VUV-MATI spectrum, adiabatic ionization energy of MVK in the ground electronic state was determined to be 9.6542 ± 0.0004 eV ($77,867 \pm 3$ cm⁻¹), which is in agreement with previous value of 9.65 eV. We performed the quantum chemical calculations at various methods and basis sets, which indicates that the ionization energies of two conformers at 298 K are almost same, implying that the 0-0 bands for two conformers in the MATI spectrum should appear at the same position. Remarkably, it was found that some twin vibrational peaks except single 0-0 band appeared in the MATI spectrum, which could be analyzed utilizing the Franck-Condon simulations and the calculated ionization onsets for two conformers of *s-trans* and *s-cis*. Herein, we ascertained the existence of the two conformers of MVK and determined their composition.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Surface-catalytic azo coupling reactions of 4-amino-4'-nitrobiphenyl on metal surface: SERS and DFT study

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Department of Chemistry, Kangwon National University, Korea

Aromatic azo compounds which exhibit important properties for critical chemical applications, have been subjected to experimental and theoretical studies from the findings of plasmon-induced azo couplings of aminobenzene derivatives. To investigate the surface catalytic photoreaction of 4-amino-4'-nitrobiphenyl (44ANBP) with two functional groups NH_2 and NO_2 , we measured the ordinary Raman and SERS spectra of 44ANBP using 632.8 nm excitation laser, which could be analyzed using quantum chemical calculations. In the SERS spectra, the characteristic peaks associated with the azo band appeared after irradiation of an excitation laser, where the vibrational peaks associated with the only NH_2 groups were found, implying that the NO_2 group in 44ANBP should be participated in the surface-catalytic photoreaction for azo coupling. However, the azo bands were not grown under acidic conditions, which indicates that the chloride ion and the proton inhibit the surface-catalytic photoreaction of 44ANBP in any way, resulting in the SERS spectrum of 44ANBP. The present study of 44ANBP possessing both amino group and nitro group on silver surface hints on mechanism of the plasmon-induced surface catalytic reaction.

Poster Presentation : **PHYS.P-145**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Cooperative Plasmon-Driven Reactions: One Reaction Helps the Other in Nanogaps

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물질의 반응성을 바꾸는 것은 화학에서의 오랜 목표이다. 본 연구에서는 나노갭 안에 두 가지 화학 반응 경로가 공존할 때, 표면 플라즈몬을 이용해 한 화학 반응 경로를 옅으로써 비활성화 되어 있던 다른 화학 반응 경로도 동시에 활성화 할 수 있음을 보이하고자 한다. 빛에 의해 유도된 표면 플라즈몬은 감쇠하면서 에너지가 높은 hot charge carrier 를 만드는데, 이를 이용하면 나노입자 표면에서 화학반응을 매우 쉽게 유도할 수 있다. 우리 연구실에서도 최근 나노갭 안에서 표면 플라즈몬을 이용해 4-mercaptobenzoic acid(MBA)의 탈카르복시 반응을 유도할 수 있음을 보이고 그 메커니즘을 규명한 바 있다. 본 연구에서는 한 발 더 나아가 MBA가 반응할 때 발생하는 hot charge carrier의 변화로부터, 반응성이 없는 분자의 반응을 새로 야기할 수는 없는지 알아 보았다. 4-nitrobenzenethiol(NBT)은 NaBH₄와 같은 환원제를 함께 넣어주고 금속 나노입자의 표면 플라즈몬을 들뜨게 할 때만 4,4'-dimercaptoazobenzen(DMAB)가 생성된다. 우리는 NBT 만을 나노갭 안에 넣었을 때는 DMAB 생성 반응이 일어나지 않으나 MBA와 mixed self-assembled monolayer를 만들어주면 염기 조건에서 MBA가 benzenethiol(BT)로 바뀌면서 (탈카르복시 반응) 동시에 NBT도 DMAB로 바뀐다(환원 반응)는 것을 발견하였다. 이는 MBA가 표면 플라즈몬에 의한 hot hole을 탈카르복시 반응에 사용하면서 hot electron의 활성도를 높이면서 그에 의한 환원 반응을 증진시키기 때문인 것으로 보인다. 우리는 이 연구를 통해 분자와 hot charge carrier와의 상호작용을 조절함으로써 특정 반응을 증진시키거나 억제하는 등의 선택적인 반응성 조절이 가능함을 보였다.

Poster Presentation : **PHYS.P-146**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile Method for Preparation of Bare Gold Nanoparticles

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금나노 입자(gold nanoparticles)는 촉매, 센서, 이미징, 치료제 등 여러 방면에 유용하게 쓰이고 있다. 특히 최근에는 금나노입자의 플라즈몬 특성을 이용하여 표면에서 화학 반응을 효과적으로 유도하는 플라즈몬-유도(plasmon-driven) 화학 반응이 주목받고 있다. 그런데 대부분의 금나노입자는 안정된 분산 상태를 유지하기 위해 표면에 캡핑 리간드(capping ligand)가 붙어 있는 경우가 많은데 이러한 리간드가 표면에서 전자 전달을 저해하여 금나노입자의 반응성을 떨어뜨리거나, 원하지 않는 부반응을 일으키는 경우가 종종 발생한다. 따라서 이러한 표면 리간드가 없는 bare 금나노입자를 만드는 것이 필요하다. 우리는 자외선 조사를 통해 리간드를 제거함으로써 bare 금나노입자를 쉽게 만드는 방법을 개발하였다. Turkevich method 를 이용해 합성한 금나노 입자의 표면에 있는 citrate를 thiol기를 가진 분자로 치환한 후에 자외선을 조사하여 나노 입자의 표면으로부터 thiol 분자를 떨어뜨린다. 이 연구에서 나노 입자는 thiol 분자와의 반응에서 안정한 모습을 보였고 자외선을 조사하였을 때 나노 입자의 표면에 결합하고 있던 분자들이 떨어져 나간 것을 라만, 제타포텐셜 등을 이용해 확인할 수 있었다. 이렇게 만들어진 표면이 깨끗한 bare 금나노입자와 리간드가 있는 금나노입자의 플라즈몬-유도 반응성을 비교 분석하였다.

Poster Presentation : **PHYS.P-147**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Validity of selection of local mode coordinates to calculate water OH stretching frequencies quantum mechanically.

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To investigate structural and dynamical properties of liquid water, OH vibrational spectroscopies have been implemented because OH stretching frequencies are very sensitive to environmental water hydrogen bond structures. Quantum mechanics(QM) is necessary to interpret many OH vibrational spectrum, and a lot of QM computational costs are mandatory. In order to calculate efficiently, mixed quantum/classical (QM/CM) methods that OH stretch mode of water molecule is selected to QM and other degrees of freedom are CM have been developed. To calculate OH stretching frequencies(potential energy surfaces; PES), many researchers have used to normal mode as coordinates but usage of local mode is reasonable and is chosen. In this work, we will show the validity of this mode.

Poster Presentation : **PHYS.P-148**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

First-principles calculations of electronic structure in nitride systems with self-consistent hybrid functional scheme

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Nitride semiconductors are good candidates which can be utilized as photovoltaic devices, light emitting diode (LED) and photocatalyst materials. In these applications, band gap properties and band edge alignments usually are the fundamental quantities since these materials require the absorption or emission of the light with appropriate wavelength range. Therefore, predicting band structure of nitrides accurately is critical for applications in life and industry. However, for density functional theory (DFT) to fail in describing band gap of semiconductor, many studies have been focused to develop methods to correct this problem. One of them is hybrid functional which mixes appropriately Hatree-Fock exchange with conventional DFT exchange-correlation functional. Despite of its better description, there is empiricism in determining Hatree-Fock mixing ratio of hybrid functional. Recently, new method that removes this empiricism was developed, called self-consistent hybrid functional[Skone *et al*, *Phys. Rev. B*, 2014, **89**, 195112]. In this study, we calculated electronic structure in bulk and surface of various nitride systems, composed of silicon, germanium, tin, gallium, aluminum, copper nitride. In addition to experimentally observed phases, hypothetical phases also were analyzed. Calculated electronic structures show more accurate results than those calculated with PBE functional and predicts the band gaps which are comparable to the high-level GW results. Our study demonstrated that self-consistent hybrid functional satisfactorily describes band structure of nitride semiconductors.

Poster Presentation : **PHYS.P-149**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Time-resolved spectroscopy with two frequency-stabilized mode-locked lasers

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Femtosecond laser has brought a dramatic development on time-resolved spectroscopy to understand the complex photochemical reactions in nature. In time-resolved spectroscopy, an impulsive pump pulse generates a non-equilibrium state, and its time evolution is monitored by a probe pulse. The time delay between the pump and probe is generated by adjusting the optical path-length difference between the two pulses conventionally. Because the experiments with mechanical time-delay have to record the data at a fixed time-delay, they require high time costs to observe slow reaction dynamics and to obtain a high resolution time-domain vibrational spectrum. Recently, we have demonstrated dual frequency-comb (DFC) based time-resolved spectroscopy. [1-2] Frequency comb being a special type of mode-locked laser has equally spaced spectral lines fixed at the frequencies specified by the laser repetition frequency and a offset frequency. When the repetition rates of two frequency combs are slightly detuned, the time-delay between them are automatically generated. The time-delay generated by DFC does not change the phase-front of the delayed beam, so that it enables wave mixing experiments such as transient absorption and two-dimensional spectroscopy even at nanosecond time delay. The use of single-point photodetector and intrinsically fast time-delay scan rate are also unique properties of DFC spectroscopy. Here, we present three DFC-based time-resolved spectroscopy, and derived them theoretically based on frequency-comb field-adapted perturbation theory. [3][1] JW. Kim, B. Cho, T. H. Yoon and M. Cho, J. Phys. Chem. Lett., 9, 1866-1871 (2018)[2] JW. Kim, T. H. Yoon and M. Cho, J. Phys. Chem. B, 122, 9775-9785 (2018)[3] JW. Kim, J. Jeon, T. H. Yoon and M. Cho, Phys. Chem., (2019)

Poster Presentation : **PHYS.P-150**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Network structure and dynamics of hydration water at zwitterionic lipid membrane surfaces

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Lipid bilayer is an excellent model system for investigating membrane structures and its hydration water. These membrane and hydration water have been studied by various experiments and computational studies. To observe detailed interactions between lipid head groups and their hydration water, we performed molecular dynamics (MD) simulation for the lipid multi-bilayer. From hydrogen bond number analysis, radial distribution, and orientational distribution of hydration water, we checked a strong interaction between phosphate group and water molecule, even to the second hydration shell. In contrast, a choline-associated water shows weak interaction with choline group. And, results from orientational relaxation and FT-IR spectroscopy for the hydration water revealed slow water dynamics and red-shifted absorption spectrum induced by the phosphate group, indicating the strong interaction between the phosphate group and its hydration water consistently. In this study, our results are in good agreement with experimental results and give insight into the interfacial water research at the lipid membrane surfaces.

Poster Presentation : **PHYS.P-151**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Crystal Transformations of Cu(I) Coordination Polymers Using Pulsed Laser Irradiation (PLI)

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Ligands (L^1 and L^2) with halogen- π charge-transfer interactions were prepared by the reaction of 3-(methylthio)propylamine and pyromellitic dianhydride/ naphthalene diimide. Coordination polymers (CPs), such as $[Cu_2I_2L^1_2]_n$ (**1**), $[Cu_2I_2L^1_2]_n$ (**2**), $[Cu_2I_2L^1]_n$ (**3**), $\{[Cu_2I_2L^1_2]CH_2Cl_2\}_n$ (**4**), and $[CuI L^2]_n$ (**5**) were synthesized by the reaction of CuI and L^1 , L^2 . CP **1** and CP **2**, dimorphic products, showed 2D network and 1D loop chain structure, respectively. CP **3** showed a 2D grid structure based on the infinite stair-step Cu_4I_4 cluster nodes. In this study, we have performed a crystal-to-crystal transformation through a pulse laser irradiation (PLI) technique. The CP powder as a target was ablated in various solutions by changing laser conditions such as its wavelength, power, and ablation time. The XRD patterns of CPs obtained correspond to that in database. Ultraviolet-visible spectroscopy and thermogravimetric (TGA) analysis were measured to confirm the spectroscopic and thermal properties of the synthesized CPs, and the structural characteristics such as morphology and size of powder particles were obtained from SEM analysis. In this work, we performed a crystal-to-crystal transformation by using the method of PLA, and resulted a new feature of our investigation including syntheses, structural characterization, and thermal properties of new copper CPs. We hope that the approach is a new and novel method for the crystal-to-crystal transformation.

Poster Presentation : **PHYS.P-152**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Computational study on the structural and thermodynamic characteristics of the Amyloid-beta peptides in Explicit Water

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The self-assembly of the amyloid- β ($A\beta$) peptides is strongly related to the pathogenesis of Alzheimer's disease. Among $A\beta$ peptide alloforms, amyloid- β 1-40 ($A\beta$ 40) and amyloid- β 1-42 ($A\beta$ 42) are the most abundant ones in the human body. Although $A\beta$ 42 differs only by the additional I41A42 residues in the C-terminus, it exhibits a greater tendency to aggregate and much higher toxicity to neurons than $A\beta$ 40. Here, we investigated the molecular factors that influence the aggregation propensity of $A\beta$ 42 and $A\beta$ 40 based on molecular dynamics simulations combined with solvation thermodynamic analyses. Although the two variants display structurally similar topologies, a slightly enhanced β -structure forming tendency is observed in the C-terminal region of $A\beta$ 42 as compared to $A\beta$ 40. The thermodynamic decomposition analysis indicates that the further dehydration of C-terminal region due to its enhanced formation of β -structure, together with two additional hydrophobic residues (I41A42), leads to the higher solvation free energy of $A\beta$ 42 relative to $A\beta$ 40. This result implies a larger water-mediated attraction between $A\beta$ 42 monomers for its self-assembly. Our results provide structural and thermodynamic understanding of the role of the C-terminal region in increasing the aggregation propensity of $A\beta$ 42 relative to $A\beta$ 40 in aqueous solution.

Poster Presentation : **PHYS.P-153**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Complex dynamics of agglomeration and dispersion of magnetite nanoparticles under magnetic field studied by measuring magnetic weight

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We have studied the dynamics of agglomeration of superparamagnetic magnetite nanoparticles by measuring the magnetic weight. The magnetic weight recorded with the electronic balance is the magnetic force that the magnetic nanoparticles experience due to the magnetic field gradient. When the sample is placed under magnetic field, the magnetic weight jumps instantaneously by the Neel and the Brown mechanisms and then increases slowly as the nanoparticles agglomerate following the stretched exponential function. The stretched exponential dynamics is observed when the involved energy barrier has a distribution. The distribution function of the energy barrier, which is determined by the inverse Laplace transformation of the dynamics, shows the maximum of ~35 kJ/mol and the width of ~8 kJ/mol. Fluctuation of the magnetic weight is synchronized with the temperature. Since the kinetic energy of the nanoparticle destabilizes the agglomerate, the magnetic weight decreases with the temperature rise, and vice versa. Thermal fluctuation is analysed by comparing the measured magnetic weight and the magnetic weight from the fitting curve which is considered as the magnetic weight at the average temperature, T_a . When it is assumed that the agglomerate of the nanoparticles is composed of many different clusters and that all the values of free energy difference between the agglomerated state and the dispersed state are allowed, the magnetic weight ratio is given by $(1 + T_a)/(1 + T)$. These results indicate that the agglomeration and dispersion of nanoparticles is a complex process which requires the energy landscape picture to understand.

Poster Presentation : **PHYS.P-154**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Quantum Chemical Study of Spectroscopy and Photochemistry of SF_5CF_3

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The molecular structure, vibration properties (IR/Raman Spectroscopy), and excited electronic energy levels of SF_5CF_3 , a greenhouse gas found very recently, was studied by combining various density-functional-theory (DFT) methods with basis sets. Because the excited states of SF_5CF_3 , reached by absorbing UV light in the upper mesosphere, could either be quenched back to the ground electronic state or dissociate to the fragments (SF_4 , CF_4 , SF_2 , F_2), we also studied the critical points on the possible pathways: the minimum energy crossing (MEX) along photo-dissociations as well as the transition state (TS) points on the ground states PES. The corresponding calculations were also carried out for the anion, SF_5CF_3^- , to study other possibilities and long-term mechanisms happening in the mesosphere

Poster Presentation : **PHYS.P-155**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Improving force fields for molecular dynamics simulations using colligative properties in physical chemistry

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In molecular biology, the conventional wisdom has been that proteins would have their defined functions by folding into highly ordered three-dimensional structures. In physical chemistry, the problem of protein folding has been an important subject over the decades. Currently, we achieved a fairly detailed view on the folding process in terms of several competing molecular interactions such as hydrogen bonds, charge-charge interactions, and hydrophobic collapses. The state-of-the-art molecular dynamics (MD) simulation method based on the physics-based atomistic model—the force fields—proved its power through the successful folding simulations of various monomeric proteins. However, as the field is moving toward new challenges—intrinsically disordered peptide (IDP) that functions without defined structures—the force fields are revealing previously unknown problems. Importantly, it turns out that the force fields overestimate most attractive forces, be they charge-charge interactions, pi-cation interactions, and hydrophobic collapses, promoting artificial aggregation of unfolded proteins. Here, we extend our years-long effort to resolve the problems using our own unique method based on physical chemistry—the NBFIX approach. In this approach, the intermolecular forces are calibrated against thermodynamic quantities such as osmotic pressure by making atom pair-specific adjustments to the non-bonded interactions. Specifically, we measure the osmotic pressure of many binary solutions of amino acid monomers and use those osmotic pressure measurements to refine the interactions between amino acid monomers. MD simulations of various IDPs show the significantly larger radius of gyration, consistent with the experimental measurements, suggesting that our refinement strategy is right on track.

Poster Presentation : **PHYS.P-156**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Computational Study on the Relationship of Hole Reorganization Energy and Electrostatic Potential Maps of Triphenylamine Based Hole Transport Materials

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Small molecule organic hole transport materials (HTMs) are widely used in electronic devices such as organic light-emitting diode, solid-state dye sensitized solar cells and perovskite solar cells. Expediting novel HTM identification for these fields, the theoretical approach aids in determining the best material. In the computational design of HTMs, the most important property to consider is the hole mobility specifically its hole reorganization energy (λ_h) component which is due to the movement of holes. It is anticipated that pinpointing the molecular part that contributes to high λ_h (more molecular distortions) would help in the efficient HTM molecular engineering by knowing which region to improve and to understand the hole transfer mechanism. Electrostatic potential (ESP) maps have been utilized to understand various chemical and physical properties. In addition, it has been shown that ESP can be a useful tool in understanding charge transfer. Hence, the relationship between the λ_h and the ESP maps of triphenylamine based HTMs has been studied. Three outcomes were drawn from the investigation: (1) the high positive potential in the ESP map of the cationic geometry is the region where more geometric distortions are occurring in going from the neutral to the cationic state, (2) large geometric distortions in this region lead to high λ_h , and (3) for tetra-substituted adamantane derivatives, delocalization of the positive potential leads to lower λ_h . The results showed that ESP maps could give insight in the molecular engineering of HTMs.

Poster Presentation : **PHYS.P-157**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Understanding NIR-to-red upconversion process of NaErF₄ and NaYF₄:Yb³⁺:Er³⁺

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Upconversion nanoparticles (UCNPs) have been widely used in various applications: bioimaging, photodynamic therapy, solid 3D displays and solar cell technology. There are several proposed mechanisms for the red, green and blue upconversion luminescence. However, luminescence mechanism of UCNPs has not been fully understood yet. Especially, NIR-to-red upconversion luminescence mechanism in NaErF₄ and NaYF₄:Yb³⁺:Er³⁺ is still in debate. In this work, the upconversion process was investigated by measuring the excitation power dependent emission spectra of NaErF₄ and NaYF₄:Yb³⁺:Er³⁺ UCNPs and by studying upconversion pathways based on one-photon and NIR multiphoton absorption. In addition, we measured time-resolved photoluminescence signals from all emission states. As such, we were able to elucidate mechanisms for green and red emissions of NaErF₄ and NaYF₄:Yb³⁺:Er³⁺.

Poster Presentation : **PHYS.P-158**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Gold Nanoparticles Ablated and Irradiated by Pulse Laser in Organic Solvents for SERS Substrate

**Seung Heon Lee, Seung Jun Lee, Talshyn Begildayeva¹, Juhyeon Park, Tae Ho Kim,
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Surface Enhanced Raman Spectroscopy (SERS) has currently investigated to analyze microscopic signals in sensors such as biosensing. In this study, we have synthesized Au nanoparticles (NPs) using ns-laser and investigated SERS effect. Au NPs are generated by ablating from the Au plate in water and acetonitrile and the solutions synthesized are irradiated without focusing by controlling the conditions of post-irradiation. Ablated Au NPs are difficult to apply to SERS substrates because their size is not uniform. However, when additional irradiation is performed, the size of Au NPs in the ns-laser is reduced and homogenized by photothermal melting-evaporation mechanisms. Therefore, we have investigated that the size and shape of Au NPs controlled in two solvents have been analyzed with Scanning electron microscope (SEM) and transmission electron microscopy (TEM), and SERS effect of Au NPs treated by laser is confirmed using Rhodamine 6G (R6G) as a target material.

Poster Presentation : **PHYS.P-159**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

NIR Porphyrin-Based Dyes for Applications in Dye-Sensitized Solar Cells

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The performance of dye-sensitized solar cells (DSSCs) is strongly dependent on the sensitizers which play a crucial role in sunlight harvesting, charge generation, and charge transport. 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 design a high-performing porphyrin-based sensitizers that harvest light up to the near-infrared region. Density functional theory (DFT) and time-dependent DFT methods were employed 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. The results obtained in this theoretical investigation provides profound understanding concerning the dye-to-semiconductor electronic interaction and charge-transfer mechanism in dye-sensitized solar cells.

Poster Presentation : **PHYS.P-160**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Real-time 2D imaging of carrier recombination dynamics of perovskite materials

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Perovskite phase is one of the promising materials for solar energy conversion application. Its high absorption coefficient, variable band-gap, and unique optical characteristics in visible spectral region enabled its conversion efficiency nearly approaching to that of Si solar cells. However, achieving durable phase under strong light irradiation and humid condition is still a challenging work. Time- and space-resolved spectroscopy is a powerful tool for the precise evaluation of photogenerated carrier recombination behavior and dynamics in perovskite phases. Until now, lifetime imaging of a frame is limited in a tens of seconds due to the scanning speed of piezo-stage. In this study, we used fast galvo scanning technique to obtain a tens of frames per second, which enabled us to study fast space-resolved carrier dynamics of perovskite materials in 2D space.

Poster Presentation : **PHYS.P-161**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Generation of ultrafast continuum mid-infrared laser pulse

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Typical pulse width of mid-IR pulse generated by OPA-dfg is limited to 200-400 cm⁻¹ which is not enough to cover whole molecular vibration region. Generation of continuum IR pulse is useful for time-resolved spectroscopy since it makes possible to observe entire vibration region with single shot. This useful broadband pulse was generated by simple colinear geometry of three pulses. Fundamental pulse passes 2 nonlinear crystals generating second harmonic and third harmonic pulse by nonlinear optical processes. Fundamental pulse with second harmonic and third harmonic pulses are focused in the air. Intense laser pulse induces the air break down into plasma. In the air-plasma, three laser pulses are mixed to generate continuum IR. Applications of continuum IR pulse would be such as multidimensional spectroscopy and IR pump-probe microscopy.

Poster Presentation : **PHYS.P-162**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Observation time-dependent mean first passage time for subdiffusive processes

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First passage times, i.e., times taken for a stochastic process to first reach a specific value are sensitive to stochastic properties of the underlying process. It is well-known that the mean first passage time (MFPT) for a particle's motion described by the fractional diffusion equation (FDE) is infinite. For a given observation time T , however, only first passage times shorter than T are used to calculate their mean value, which is always finite. For three different kinds of subdiffusive processes, i.e, FDE motion, scaled Brownian motion (SBM), and fractional Brownian motion (FBM), where their mean square displacements in the absence of boundaries are the same as each other, the T -dependent MFPTs for a particle freely moving in an interval $[-L,L]$ are compared with respect to their dependences on L and T . The relationship between such dependences of the MFPT and stochastic properties of the underlying process are also discussed.

Poster Presentation : **PHYS.P-163**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Axial Ligand Dependent MO Interactions along the Reaction Coordinates of Hydrogen Atom Transfer in the C-H Activation by P450 Cpd I.

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Cytochromes P450 catalyzes a range of different oxygen atom transfer reactions in nature. The axial ligand plays an important role in the reactivity of Iron(IV)-oxo porphyrin π -cation radical complexes in enzymatic and catalytic hydroxylation reaction. To elucidate the axial ligand effect in Iron(IV)-oxo porphyrin complexes, we have performed a series of density functional theory calculations on the hydroxylation of ethane by $[\text{Fe}^{\text{IV}}=\text{O}(\text{Por}^{(\cdot+)})\text{L}]$ (Por=Porphyrin ring, L= SCH_3^- , OCH_3^- , imidazole, etc), which afford ethanol product. Three spin states of $[\text{Fe}^{\text{IV}}=\text{O}(\text{Por}^{(\cdot+)})\text{L}]$ (Doublet, Quartet, Sextet), of each ligands were considered and the reaction coordinate H-transfer were calculated. The spin-dependent orbital interactions between the axial ligand of iron-oxo porphyrin system and substrate were monitored along the reaction coordinate, and the results in reaction to the catalytic activity will be presented.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spectroscopic properties of BODIPY aggregates

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Liquid phase organic laser dyes have spatial limitations and inconvenience of medium management. Therefore, the need for solid phase lasers emerged. But for solid phase organic laser dyes, medium stability is important. BODIPY(difluoroboron dipyrromethene) derivatives have short stokes shift and variable absorbance, emission wavelength and good photostability. BODIPY derivatives can be self-assembled in high water fraction solution. Most of the emission intensity of organic nanowires decreases as they become aggregates. However, BODIPY aggregates have aggregation induced enhanced emission property. Since these aggregates are made in the form of nanowires, they can act as favorable lasing cavities. BODIPY nanowires show amplified spontaneous emission property and act like Fabry-Perot cavity at solid phase.

Poster Presentation : **PHYS.P-165**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Direct observation of phonon dynamics of metal thin film

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Visualization of chemical reactions is one of the ultimate goals in chemical dynamics of isolated molecules, liquids and materials.[1-3] Ultrafast Electron Diffraction (UED), a member of 4D electron imaging apparatus, is a toolkit to film the snapshot of transient structures during the bond dissociation or formation. Recently we have introduced RF compressing technique to bunching the electron beam which is a promising tool to get the hundreds of femtosecond electron pulse duration in the laboratory-scale machines. Due to this compression technique, measuring the time-duration of bunch also have been one of the most important steps in manipulating the UED setup. UED apparatus in IBS is designed for sub-Å (spatial) and sub- picosecond (time) resolution in single shot. UED apparatus in IBS mainly consists of three parts: 1) electron gun driven by 90 keV accelerator and Ti:Sapphire femtosecond laser system, 2) RF-based electron beam compressor and 3) detector assembly to measure the diffraction pattern as a function of delay time. 100 keV accelerated electron beam generated by tripled output of Ti:Sapphire femtosecond laser output (800 nm, 1 kHz, 35 fsec) fly to the RF-compressor to re-compress the lengthened electron pulse duration flying. The diffraction patterns for transient structures are obtained by pump(laser)-probe(electron) scheme. Time synchronization between RF-compressor and electron beam is achieved by Phase-Locked Loop (PLL) device. With this apparatus, metal thin film systems (sub 30 nm) were measured and lattice coupled phonon dynamics were clearly observed. The obtained experimental diffraction data are integrated and analyzed to get the structural information as a function of time delay between pump laser and electron beam. References[1] Miller, R. J. D., Science 2014, 343, 1108.[2] Chergui, M., Zewail, A. H., ChemPhysChem 2009, 10, 28.[3] Weber, P. M. et al. J. Appl. Phys. 2005, 97, 111101.

Poster Presentation : **PHYS.P-166**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The Li ion battery's electrolyte solvation dynamics in operando condition

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Electrolyte is one of the main components of lithium ion batteries and consist of solvent salts and additives. The electrolyte plays a role as a transport channel for lithium ions and is closely related to battery performance such as charge rate, capacitance, stability, and safety. In the currently commercialized lithium ion battery, the electrolyte is formed by dissolving a lithium salt in a mixed solvent of cyclic carbonate and linear carbonate. The cyclic carbonate has a high dielectric constant to stabilize the Li cation, and the linear carbonate has low viscosity to help transport the Li cation. Many previous studies have dealt with bulk electrolytes that are not applied potential. However, it is very important and necessary to observe the solvation dynamics in operando condition to understand the operation mechanism of the lithium ion battery. By measuring FT-IR with home-built spectro-electro-chemical cell, it was observed that the electrolyte near the electrode had a different solvation dynamics than the bulk electrolyte.

Poster Presentation : **PHYS.P-167**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Morphological Changes of Tandem Organic Photovoltaics

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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 have found that an effective way to improve OPVs is to use a tandem structure. Tandem OPVs provide a way to harvest the broader spectrum of solar radiation by combining two or more OPVs systems. So, in this study, we made a tandem structure composed of two layers. One layer was composed of Poly([2,6'-4,8-di(5-ethylhexylthienyl)benzo[1,2-b;3,3-b]dithiophene]{3-fluoro-2[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl}) (PTB7-Th) as a donor and 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(5-hexylthienyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC-Th) as an acceptor. The other layer was composed of Poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)) (PBDB-T) as a donor and [6,6]-Phenyl-C71-butyric acid methyl ester (PC70BM) as an acceptor. We then investigated the effects of the tandem structure on the morphological changes of the tandem OPVs by examining the movements of the acceptors ITIC-Th and PC70BM when the order of the two layers was altered.

Poster Presentation : **PHYS.P-168**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spectroscopic studies of jet-cooled 6-cyanoindole : R2PI, IR-dip and UV-UV hole-burning spectroscopy

Wooyeong Kim, Cheol Joo Moon, Hak Seung Ryu¹, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

¹*Gyeongsang National University, Korea*

In this work, we measured the excitation spectra of jet-cooled 6-cyanoindole by mass-selected resonant two-photon ionization (R2PI), infrared-dip and UV-UV hole-burning spectroscopy in a gas phase experiments. R2PI spectrum of the 6CI monomer was obtained in the frequency range of 31000~35000cm⁻¹. The peak at 33459cm⁻¹ was founded to be the origin transition of the 6CI monomer. We investigated conformational information of the 6CI monomer by fixing the pump laser at the origin band and scanning the probe laser(using the UV-UV hole burning technique). The observed IR-dip spectrum was compared with the predictions done by the density functional theory (DFT) calculations with a 6-311++G(d,p) basis set.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The electronic spectroscopic studies of jet-cooled 2-cyanoindole and its water clusters: R2PI and computational calculation.

Hak Seung Ryu, Wooyeong Kim, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

In this study, 2-cyanoindole (2CI) has found some spectroscopic interest about excited state in the gas phase. The excitation spectra of 2-cyanoindole (2CI) and its water clusters, $2\text{CI}-(\text{H}_2\text{O})_n$ ($n = 1\sim 3$), have been measured by using mass-selected resonant two-photon ionization (R2PI) in the gas phase. For monomer, R2PI spectrum was obtained, but with a broad spectral feature. However, it was possible to observe sharp spectral peaks for $2\text{CI}-(\text{H}_2\text{O})_{1-3}$ clusters upon adding water. Moreover, the origin band of each cluster shifted to the red frequency as the number of water increased. The transition energy of the origin band of the R2PI spectrum was compared with that obtained by density functional theory (DFT) calculations. To further investigate the $2\text{CI}-(\text{H}_2\text{O})_{0-3}$ systems, we have employed the various gas-phase spectroscopic techniques, such as, UV-UV hole burning (UV-UV HB) and IR-dip spectroscopy.

Poster Presentation : **PHYS.P-170**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Construction of pH-Sensitive Upconverting Luminescent Nanoparticles

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Detection of pH at the intra-cellular level is of great importance to solve the concerned questions in biomedical research and it is still challenging to devise appropriate pH nanoprobe for pH determination under near-infrared excitation. Despite the fact that the upconversion nanoparticles in imaging and drug-delivery have been explored thoroughly, the investigation on their application in pH-probing has not been dealt with comprehensively. Herein, we report a rationally designed upconversion system that combines a core with double shell layers conjugated to fluorescein dye molecules and its pH sensing ability upon two near infrared laser light excitations. The energy migration processes and mechanism of upconversion, involved within the spatially separated lanthanide ions in the nanostructure have additionally been illustrated. In the designed sensor, one upconversion luminescence band shows variation with pH due to absorption of that light by the conjugated fluorescein molecules while the bands at other regions remain unchanged. Thus, the self-referenced, ratiometric sensor was constructed upon longwave light excitations with inner filter effect.

Poster Presentation : **PHYS.P-171**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Vibrational circular dichroism spectroscopy of jet-cooled ephedrine and its hydrated clusters

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Department of Chemistry, Chungbuk National University, Korea

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 determine absolute configurations of chiral molecules. Especially, the CD values of the OH stretching vibrational mode show significant differences among different conformers because the vibrational modes of hydroxyl groups reflect the structural environment. Here, we obtained the VCD spectra of the hydrated clusters of Ephedrine(ED) in a supersonic jet using IR-UV double resonance spectroscopy. The hydrated clusters of ED in a supersonic jet were irradiated with a circularly polarized IR laser pulse and then a linearly polarized UV laser pulse for resonance-enhanced two photon ionization (R2PI). 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 the hydrated clusters of (-)-ED and (+)-ED near the OH stretching vibrational band. In these spectra, the OH vibrational modes of the water molecule bound to ED show the induced CD effects through the hydrogen bonding interaction with ED. Theoretical calculations using TDDFT at the M06-2X/6-311++G(d,p) level was carried out to predict the CD values. These results are the first induced VCD values of hydrated clusters in a supersonic jet. We will discuss the chirality transfer from a chiral molecule to an achiral molecule and the mode dependence of induced VCD phenomena.

Poster Presentation : **PHYS.P-172**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Correcting Approximate Density Functionals by Parts

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Present density functional theory (DFT), although their successful estimations of equilibrium geometries and energies, most of the approximate functionals suffer predicting energies of non-equilibrium geometry complexes. Previously, we show that using Hartree-Fock (HF) electron densities to calculate DFT energy (HF-DFT) of non-equilibrium geometry complexes gives remarkable improvement with respect to self-consistent DFT. Here, we analyzed this phenomenon by decomposing the total energy error into a density-driven part (density-driven error) and a functional-driven part (functional error). Using Kohn-Sham inversion technique, a fairly accurate electron density can be put into approximate density functionals and help accurate decomposition of density-driven and functional error. By the error classification by parts, we show that the use of HF density cures DFT energy errors in two ways without introducing additional empirical parameters; corrects the density error of the self-consistent density when the functional error is negligible or cancels the delocalization error present in the approximate functionals.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Accurate Description of Torsional Energy Profile using Density-Corrected Density Functional Theory

Eunbyol Cho, Eunji Sim*

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When performing approximate density functional theory (DFT) calculations, density-driven errors are caused by inaccurate self-consistent densities and can be reduced using better densities rather than approximate densities. Density-driven errors have a significant impact on the accuracy of density functional calculations not only for strong interactions such as covalent or ionic bonds but also for weak interactions including torsional rotations. The torsional energy profile caused by intramolecular rotations requires an electron density that can accurately represent subtle changes due to torsional angles. However, self-consistent DFT densities result in an inaccurate torsional energy profile due to the delocalization error that causes the density-driven error. Here, we examined ten approximate density functionals for the data set of glyoxal and its derivatives. In this data set, self-consistent DFT calculations are inaccurate and unreliable because they sometimes predict wrong equilibrium conformations. We show that the density error causes such inaccuracies and the density-corrected calculation of HF-DFT, which evaluates the DFT energy on Hartree-Fock density, not only reduces the error of torsional barriers by half but also achieves precise torsional energy profiles at all angles.

Poster Presentation : **PHYS.P-174**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Heterogeneous OER catalytic reaction study using in situ Sum-frequency generation spectroscopy

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Water oxidation is an essential reaction for energy storage such as forming of hydrogen or hydrocarbons without accumulation of by-product. Unfortunately, This reaction is consist of a complex multistep, which adds a considerably large overpotential to the actual process. Although many studies have been conducted on OER catalysts with low overpotential and high stability, the specific catalytic reaction mechanism has not yet been elucidated. To understand the nature of heterogeneous catalytic reaction mechanism, it is important to use surface/interface selective spectroscopic method. Here, using vibrational sum-frequency generation (VSFG) spectroscopy, we selectively identified electrode-electrolyte interfacial molecules. And we designed spectro-electrochemical (SEC) cell for in situ SFG experiment. In this work, using nonlinear spectroscopic method, we can observe that the hydrogen bonding network of the interfacial water molecules changes at each potential.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Observation of changes in the morphology and bulk phases of TiO₂ nanoparticles under pulsed laser irradiation in water

HeeJun An, Youngdong Yoo¹, Yu Kwon Kim¹, Hyuk Kang^{1,*}

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Titanium oxide (TiO₂) is used in diverse area such as solar cell, photocatalyst, and sensor due to its good photoresponsive properties. TiO₂ has a relatively large band gap (3.0 ~ 3.2eV) which can respond to a prevalent ultraviolet (UV) light of a solar spectrum (5% of the sunlight). Interestingly, the detailed photoresponsive characteristics of TiO₂ can be tuned in a number of different ways by controlled changes in its shape, type of bulk phases and the introduction of defects in the bulk as well as on the surfaces. Here, the preparation methods and the post-treatment techniques have a huge influence on the ultimate photoresponsive properties of TiO₂. One way to tune the properties of TiO₂ is to use a laser irradiation directly onto TiO₂ nanoparticles dispersed in water. Earlier, it has been reported that black TiO₂ can be prepared from white TiO₂ powders by 532 nm nanosecond laser pulses. However, it is a still open question on how visible light can be absorbed by TiO₂ which can only respond to UV light. Thus, in this study, we studies structural changes of TiO₂ powders in water under the irradiation of nanosecond laser pulses of 532 and 1064 nm. We find that in both cases (532 and 1064 nm) TiO₂ can change its color from white to grey suggesting that some changes responsible for the apparent color occur on TiO₂. But the detailed investigation on the bulk phases (by XRD) and the morphology (by TEM) revealed that the initial bulk phases and the overall shape of TiO₂ nanoparticles are preserved. Instead, additional nanostructures on the TiO₂ nanoparticles were observed. We believe this small finding will pave a way to a better understanding on the mechanism of laser pulse-induced changes of TiO₂.

Poster Presentation : **PHYS.P-176**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Identifying phosphorylation site of Janus kinase 3 using cryogenic ion spectroscopy of DYYVVR

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Protein phosphorylation is an important post-translational modification, which usually occurs in the OH functional group of tyrosine, serine, or threonine in a protein. Above all, phosphorylation of tyrosine plays a significant role as signal transduction in a cell. Numerous researches have been conducted to find how such phosphorylation happens. For example, a research that uses antibody PY20, which perceives tyrosine in the protein, can tell if this amino acid is phosphorylated or not through SDS PAGE and western blotting. These methods are comparatively easy ways to find the phosphorylated tyrosine, however, is not suitable for investigating which tyrosine is the phosphorylation site in the protein. We aim to find out the phosphorylation site of a peptide containing tyrosine residues by means of cryogenic ion spectroscopy in the UV region. One of tyrosine kinases, Janus kinase 3 (JAK3) has Y980 and Y981 (980th and 981st tyrosine residues), where Y980 positively regulates its kinase activity and Y981 negatively regulates itself. A tryptic peptide of JAK3, JAK3979-984, contains both Y980 and Y981 and has the sequence of DYYVVR. We conducted a UV photodissociation spectroscopy of protonated DYYVVR, DFYVVR (Y980F), DYFVVR (Y981F), DpYYVVR (Y980 phosphorylated), DYpYVVR (Y981 phosphorylated), and DpYpYVVR in a cold ion trap. The two tyrosine residues showed well-separated UV absorption bands, and each phosphorylation was easily differentiated. We also identified conformers of these peptides by UV-UV or IR-UV hole burning spectroscopy.

Poster Presentation : **PHYS.P-177**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Ultrafast Infrared Spectroscopy Study of Azides with β -isotope labeling: Comparing with Aliphatic Azides and Aromatic Azides.

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Azides can be used as infrared (IR) probes of the local environment and molecular structural changes. The dynamics reported by a site-specific IR probe is limited to its vibrational lifetime, restricting the utility of azide probes due to short vibrational lifetimes. Moreover, the vibrational bands of azide probes are often accompanied by complex line shapes that arise from Fermi resonance. If these limitations could be overcome, their strikingly large molecular extinction coefficients would make azide groups very attractive as IR probes. We have synthesized primary and aromatic azides, and performed Fourier transform infrared (FTIR) and nonlinear infrared experiments (IR pump-probe and 2D-IR) to determine changes in azide stretch vibrational modes associated with isotope labeling, with the hope of avoiding Fermi resonance and increasing vibrational lifetime. Based on our FTIR results, ^{15}N isotopic labeling did not effectively modulate azide stretching frequency from accidental Fermi resonance. 2D-IR spectra measured due to check the fermi resonance. There are cross-peak in aromatic azides. These cross-peaks mean that two vibration bands are involved in Fermi resonance. vibrational relaxation dynamics does not follow the same pattern when isotope labelling aliphatic and aromatic azide probes, respectively. All azide derivative 1-2 transition frequencies show a blue-shifted over time. We found that the azide stretches overlap with combination modes, by time-resolved IR-PP spectra. Our study lays groundwork for the research on new IR probes involving the isotope labeling of azide probes.

Poster Presentation : **PHYS.P-178**

Physical Chemistry

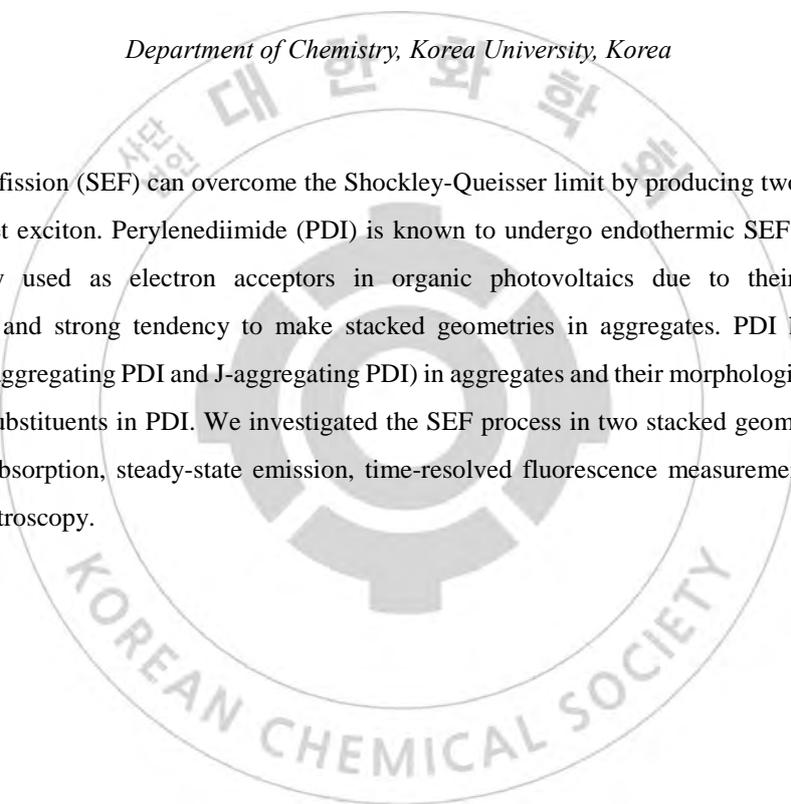
Exhibition Hall 2, FRI 11:00~12:30

Singlet exciton fission in two stacked geometries of perylenediimide

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Singlet exciton fission (SEF) can overcome the Shockley-Queisser limit by producing two triplet excitons from one singlet exciton. Perylenediimide (PDI) is known to undergo endothermic SEF in films. PDI is also commonly used as electron acceptors in organic photovoltaics due to their photostability, thermostability and strong tendency to make stacked geometries in aggregates. PDI has two stacked geometries (H-aggregating PDI and J-aggregating PDI) in aggregates and their morphologies are controlled by side-chain substituents in PDI. We investigated the SEF process in two stacked geometries of PDI by using UV-vis absorption, steady-state emission, time-resolved fluorescence measurement, and transient absorption spectroscopy.



Poster Presentation : **PHYS.P-179**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Cooperative protein structural changes of homodimeric hemoglobin arising from weakened network of subunit interface studied by time-resolved X-ray solution scattering

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Homodimeric hemoglobin, HbI, is an excellent model system of allosteric effect and cooperativity. In an effort to expand previous studies with time-resolved X-ray solution scattering (TRXSS) on wild-type, F97Y, and T72V mutant HbI, here, we conducted TRXSS experiment on the K30D mutant to elucidate the kinetics and structural information such as rotation angle and heme-heme distance in the time range from 100 ps to 10 ms. The K30D mutant lacks the salt bridge located in the subunit interface of the wild type thereby the attractive force of dimeric interface being weakened compared with wild type. Unlike the wild type, the K30D mutant contains a significant portion of monomers in addition to dimers due to the weakened interaction between the two subunits. We built the kinetic model considering five time constants with four structurally distinct intermediates containing the monomer. Considering that the time constant of the K30D mutant was larger than that of wild-type in transition of from I2 to I3 of dimer, the weakened interaction between the two subunits may be involved in controlling rate of the quaternary structural changes which occur in biphasic transition. In addition, another major structural change is that I3 intermediate of the K30D mutant is formed via subunit rotation and an increase in the heme-heme distance during the transition from I2 to I3 of dimer. The heme-heme distance of all intermediates of the K30D mutant was 0.53 Å longer than that of wild-type, suggesting that the salt bridge plays an important role in stabilizing the entire quaternary structure of HbI. The tertiary structural change was also greatest in the I2 to I3 transition, and the degrees of freedom of the helices near the D30 and D89 residue, which was no longer involved in the salt bridge, were larger than those of the wild-type. By comparing the structures of protein intermediates in wild-type HbI and the K30D mutant, we elucidated how the salt bridge in the subunit interface affects the kinetics and structures of reaction intermediates of HbI.

Poster Presentation : **PHYS.P-180**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The reaction mechanism study for the synthesis of benzoxazole with Flow cell and Two-dimensional correlation method

Yeongseok Chae, Chaiho Lim, Kyungwon Kwak*, Minhaeng Cho*

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Highly efficient synthesis of benzoxazole from Schiff bases of 2-aminophenol with aldehydes was introduced by Cheon's group in 2012. Since benzoxazole is a building block commonly used for biologically active materials and the synthesis is under mild condition without the use of any external metal co-oxidants, there were interest and controversy in the mechanism of the reaction especially the order of oxidation and cyclization. There are three main steps in the reaction. First one is that cyanide, catalyst, attacks an imine group of aniline and proton transfer occurs neutralizing the intermediate. Next, SN2 cyclization reaction occurs. After hydroxyl group loses a proton, oxide attacks a carbon to which the nitrile group is bonded. Finally, after dihydrobenzoxazole is formed, oxygen in air removes two protons of the intermediate and benzoxazole, product of the reaction, is formed. This process was hypothesized by Cheon's group at first. However, Chen et al. in Nankai University refuted the mechanism with DFT calculation asserting that oxidation should precede to cyclization reaction. In situ IR study was performed with flow cell and the intermediates were observed in IR spectra in spite of very small intensity. They were double checked by 2D correlation method that shows the order of peaks over time. We believe that the mechanism was confirmed.

Poster Presentation : **PHYS.P-181**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Dual frequency comb spectroscopy for optical activity measurement

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We present a novel application of dual frequency comb (DFC) spectroscopy for optical activity measurement of chiral molecules in condensed phase. To do this, we propose to apply the linear DFC spectroscopy technique for the measurements of two orthogonal polarization components of the linearly-polarized OFC transmitted through the optical sample. By measuring two interferograms corresponding to the horizontally- and vertically-polarized transmitted electric fields, the difference of the complex susceptibility spectra between left and right-circularly polarized field can be obtained. The DFC interference signals in each polarization components will be transformed into the frequency domain by a FFT method to get the imaginary and real parts of the susceptibility spectra for the circular dichroism (CD) and circular rotatory dispersion (ORD) measurements. In this study, we consider the optical activity measurement of a metal complex of Ni-(±)-(tartrate)₂ by using identical broad-band OFCs from Ti:Sapphire mode-locked laser around 800 nm with 80 MHz repetition rate and 7.5 fs pulse-width. We anticipate that the CD/ORD spectroscopy with dual frequency comb proposed in this study can be extended to time-resolved CD/ORD spectroscopy of extremely weak CD values, which has been experimental challenges for long time.

Poster Presentation : **PHYS.P-182**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effects of the spatial arrangement of nanoparticles on the glass transition temperature of polymer fibers

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Introduction of nanoparticles (NPs) into polymeric systems has been used to control the glass transition temperature (T_g) of polymeric systems. Previous studies showed that the interaction type of NPs is one of the crucial factors in determining T_g of polymeric systems. Also, previous experiments revealed that the spatial arrangement of NPs in confinement polymeric systems, like polymer films and fibers, affects T_g of polymeric systems. However, such effects of NPs on the glass transition temperature are yet to be understood at a molecular level. In this work, we perform molecular dynamics simulations for polymer fibers and polymer melts with NPs of different types of intermolecular interactions. We investigate the glass transition temperature of polymer fibers and melts. We illustrate that, upon the addition of NPs, the effects of the interaction types of NPs in polymer fibers are different from that of the interaction types of NPs in melts. Adding NPs with attractive interactions into melts increases T_g of polymer melts, whereas adding NPs with relatively repulsive interactions into melts decreases T_g of polymer melts. On the other hands, adding NPs into polymer fibers increases T_g of polymer fibers regardless of the interaction types of NPs. We also find that the interaction types of NPs determine the spatial arrangement of NPs in polymer fibers. NPs with relatively repulsive interactions are located at the surface of polymer fibers, which causes decreasing the mobility of monomers at the surface of polymer fibers and increasing T_g . In the case of polymer melts, NPs with relatively repulsive interactions cause increasing the mobility of monomers and decreasing T_g .

Poster Presentation : **PHYS.P-183**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Adsorption and Desorption Properties of CNT-sponge Preconcentrator

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Carbon nanotube sponge (CNTS) was fabricated using a spray pyrolysis CVD and tested as an adsorptive material of a thermally desorbed preconcentrator for GC analysis. Direct current flow through the porous CNTS allows rapid thermal heating (264.7 °C with a 481.5 °C/s rate), narrow desorption (0.74 s), and >96% desorption efficiency. The preconcentrator exhibited low detection limits of part-per-trillion level, low affinity against humidity, and good repeatability under optimized conditions. Thus, CNTS preconcentrator has potential for use in fast and accurate real-time analysis of VOCs in ambient air and gaseous samples, in which the enriched vapors are desorbed to a various analytical device, such as a gas chromatograph, mass spectrometer, or sensor array for detection.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Molecular Dynamics Study for the Effect of Additive Ions on Phase Transformation of Amorphous Precursor Phases of CaCO₃

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Calcium carbonate is an earth-abundant material that exists in a variety of natural environments, including soils and sediments. In recent years, amorphous calcium carbonate (ACC) phases has increasingly received scientific attention because their local orders in the short-range can determine the subsequent pathways for phase transformation. However, the fundamental understanding about the structure-property relationship for these amorphous precursor phases is still lacking. As a fundamental work to elucidate this issue, we introduced additive metal ions, which are usually soluble in aqueous solution and can tailor the local orders of ACC with different hydrophilicity. With molecular dynamics simulation, we investigated the effect of additive ions on the phase transformation process of the ACC model system by varying the hydration levels and molar compositions of additive ions (i.e., Mg²⁺, Fe²⁺, Ba²⁺ and Sr²⁺). Starting from the cluster nucleation in aqueous solution, the hydrated and anhydrous forms of ACC were systematically examined following the dehydration scheme. Our results revealed that additive ions can exert promoting or inhibiting effect depending on their different hydration strengths and ionic radius. These results can provide a valuable information for controlling the structure and stability of amorphous precursor phases, which can shed light on the mineral carbonation processes for CO₂ capture.

Poster Presentation : **PHYS.P-185**

Physical Chemistry

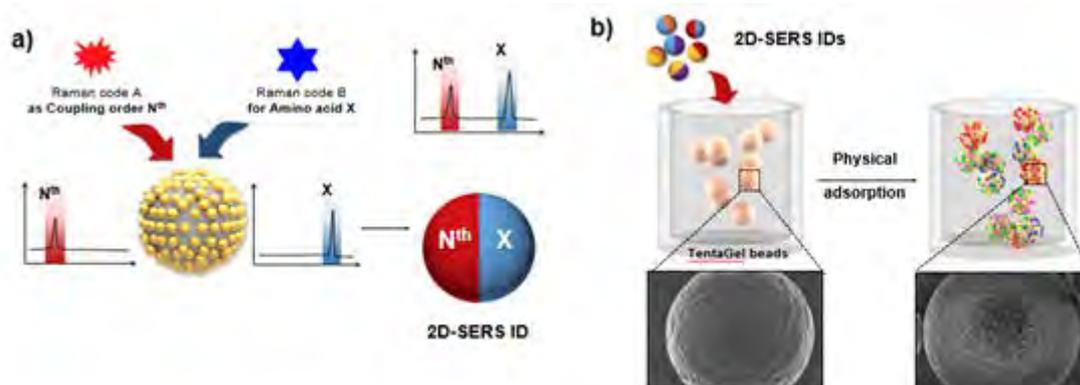
Exhibition Hall 2, FRI 11:00~12:30

Two-Dimensional Raman Encoding System for Combinatorial Peptide Libraries with High-Throughput Assay

Sung Gun Lee, Dae Hong Jeong*

Department of Chemical Education, Seoul National University, Korea

The combinatorial chemistry is widely utilized to prepare an extensively large number of combinatorial libraries for drug discovery and peptide profiling. To efficiently identify a leading compound in combinatorial libraries, a simple and reliable encoding/decoding method involving bio-assay is essentially required. Here, we developed a simple, efficient, and reliable on-bead peptide sequencing method using two-dimensional Raman labeled surface-enhanced Raman scattering nano-identifiers (2D-SERS IDs). By encoding two-dimensional SERS codes: coupling step codes and amino acid codes, a sufficiently large number of unique SERS codes could be generated that enough to encode every possible combinatorial peptide with a small number of Raman label compounds. The 2D-SERS IDs were physically attached on microcarriers and were readily identified by single Raman mapping. Through this strategy, the affinity of peptide ligands on the beads to streptavidin was successfully screened. We believe that the 2D-SERS IDs encoding method can be utilized to rapidly and reliably screen in a huge number of combinatorial libraries for drug discovery.



Poster Presentation : **PHYS.P-186**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A portable GC for real-time monitoring of VOCs in air samples

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Department of Chemistry, Wonkwang University, Korea

Current study describes a portable GC (30×26×15 cm³, 5.5 kg) for field determination of trace levels of organic mixture vapors. This system is comprised of a CNT-sponge preconcentration sampler, a capillary column module with at-column heater configuration, an electronic pneumatic control of filtered/pressurized ambient air as a carrier gas, and a photo ionization detector (PID). A tablet computer was embedded to perform a stand-alone operation that can provide both instrument control and chromatogram data handling without an external computer. Based on the experimental results, the system can effectively separate and detect the trace amount of air pollutants within 10 min. The results show that this portable GC-PID can be widely applied to the on-site detection, including indoor air quality, industrial emission control, rapid detection of explosives in public place, and breath analysis.

Poster Presentation : **PHYS.P-187**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

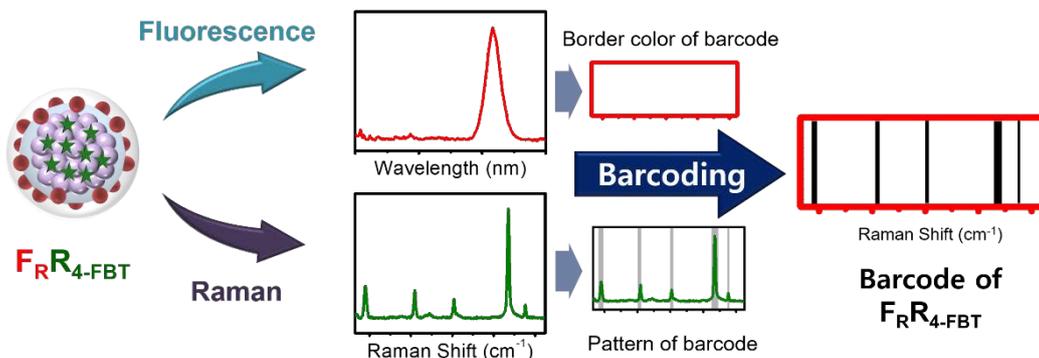
High-throughput Multiplex Analysis Method Based on Fluorescence-SERS Quantum Dot Embedded Silver Bumpy Nanoprobe

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Developing multiplex detection and analysis with spectroscopic technique using SERS-based dual modal nanoprobe is important issues for applying biological encoding, multiplex biomarker imaging and immunoassay technique. In this paper, we fabricated fluorescence-SERS dual modal quantum-dot (QD) embedded silver bumpy nanoparticles for high-throughput multiplex analysis tool. Using 15 kinds of silica-coated silver bumpy nanoshells (AgNS@SiO₂) with different Raman label compound and 3 kinds of QDs (red, green and blue), total 45 kinds of dual modal nanoprobe (FRGBRSERS) were prepared. Each FRRSERS nanoprobe has strong SERS and fluorescence signal for analyzing multiplex signal. Based on this dual modality, we propose a barcode-based machine learning algorithm method that transforms spectra into barcodes and identifies the chemical information with the barcodes. As a proof-of-concept we carried out a model experiment to identify both a single label spectra and triplex label spectra from 15 kinds of Raman labels library. Our developed FRRSERS and high-throughput multiplex analysis algorithms have huge potential at developing multiplex detection platform for analyzing and encoding biological target.



Poster Presentation : **PHYS.P-188**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Adsorption behavior of cis-2-butene-1,4-diol on Ge(100)

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Chemical reaction of cis-2-butene-1,4-diol with Ge(100) surface was investigated using density functional theory (DFT) calculations. Our calculation elucidated the competition and selectivity between reactive functional groups of cis-2-butene-1,4-diol on Ge(100) 2×1 surface. The most stable configuration involved the dual OH-dissociation of cis-2-butene-1,4-diol molecule, followed by the formation of dual Ge-O bonding. The bridged structure between two surface Ge atoms had Ge-O-C-C-C-C-O-Ge linkage. The dissociated H atoms were also bonded to other surface Ge atoms. Our simulated images of the stable adsorption structures contained characteristic features due to electronic charge density around the reacted surface.

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Silver Nanoshell: One-step, Surfactant-free Controlled Synthesis for Regulating Surface Morphology and Their Enhanced Scattering Properties

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Using surfactants like cetyltrimethylammonium bromide (CTAB) and introducing seed-mediated synthesis process has been general way to control surface morphology of nanoshell [1]. However, studies using these methods face went through several problems such as excessive amount of bulky surfactants needed in the reaction and time-consuming multi-step processes. In this poster, we presented single-step and surfactant-free synthesis which can control morphology as well as thickness of silver nanoshells with alkylamines. As alkylamines, butylamine, octylamine, dodecylamine, hexadecylamine, ethanolamine, propanolamine and tributylamine were used as reductant and capping agent. We studied on effects of alkyl chain length, existence of hydroxyl group, and the degree of alkyl chain in silver shell formation, which results in change on surface morphology and thickness of silver nanoshell. Several factors such as reduction speed, steric effect, reducing power of the alkylamine contribute to this changes. Confirming the enhanced scattering properties of synthesized silver nanoshell with different surface morphologies, we investigated optical properties of each silver nanoshell by observing Surface Enhanced Raman Scattering (SERS) at the single particle levels. According to nanoshell surface morphology, intense and uniform SERS signal was detected for single particle and their SERS enhancement factor for each particle were calculated up to ~107. REFERENCES[1] Sanchez-Gaytan, B. L.; Qian, Z.; Hastings, S. P.; Reza, M. L.; Fakhraai, Z.; Park, S.-J. The Journal of Physical Chemistry C 2013, 117, (17), 8916-8923

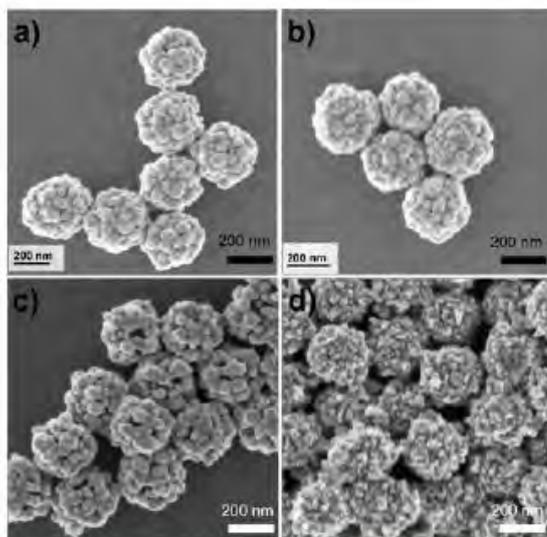


Figure 1 TEM images of (a) BNS, (b) ONS, (c) DNS and (d) HNS

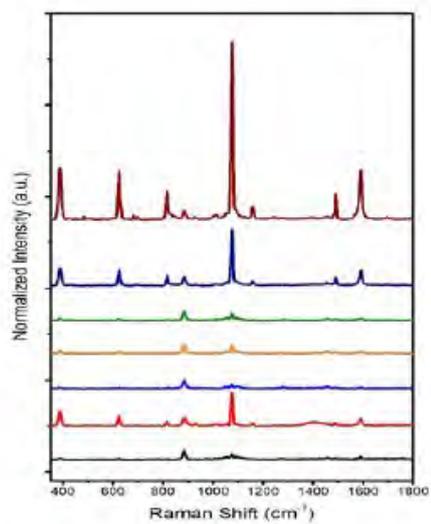


Figure 2. SERS spectra of the 4-FBT spectra obtained from 660 nm excitation on each 7 of AgNSs

Poster Presentation : **PHYS.P-190**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Molecular dynamics studies on rotator-solid phases of imidazolium-based organic ionic plastic crystals

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Organic ionic plastic crystal (OIPC) is a unique solid phase that exhibits rotational disorder while ions maintain a long-range ordered 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-191**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Observation of field-molecule interaction in REMPI spectrum of polyatomic molecule

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In spectroscopy, strong interactions between dipole transitions and oscillating optical fields has been known to induce spectral phenomena such as a shift or a splitting of spectrum. Especially for AC Stark effect, the experiments and theoretical investigations has been well established and interpreted by many chemical physicists for a century. However, the researches on the AC Stark effect have quite limited ranges such as single atoms, metal dimers, and diatomic molecules since it requires strong dipole transitions between well-resolved quantum states leading significant coherent Rabi cycles. Recently, we have observed unexpected field-molecule interaction between ns laser pulse and 2-methoxythiophenol (2MTP) molecule which has more than 10 atoms. The origin peak of S1 state REMPI spectrum of 2MTP turns out to be split into two parts at high energy of laser pulse and the amount of splitting is directly proportional to the magnitude of given laser field. Changing the excited state lifetime by substituting deuterium on SH group also affect on the amount of splitting and linewidth(lineshape), so we conclude AC Stark effect occurs on this system. Semi-classical spectrum calculation using decay-associated two-level dressed state model successfully interprets our experimental results.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of size and shape of TiO₂ nanoparticles on charge carrier dynamics

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Department of Chemistry, Sungkyunkwan University, Korea

Investigation of charge carrier dynamics is essential to understanding and enhancing the efficiency of photochemical reactions catalyzed by TiO₂. In this study, we carried out nonadiabatic molecular dynamics simulations combined with real-time time-dependent density functional theory to investigate the effects of size and shape on charge carrier dynamics in TiO₂ nanoparticles (NPs). Using the Wulff construction method, we constructed both octahedral (10, 35, and 84 TiO₂ units) and cuboctahedral (29, 78, and 97 TiO₂ units) nanoparticles with size varying from 1 to 3 nm. Generally, the recombination rates decreased with increasing NP size. The relaxation time increased with increasing NP size, as the nonadiabatic coupling (NAC) and exciton binding energy (ΔE_{ex}) decreased. The cuboctahedral NPs showed smaller ΔE_{ex} compared to the octahedral NPs. For the octahedral NPs, the smaller NAC and shorter dephasing time contributed to longer relaxation, despite smaller transition energy, as the size increased. However, the influence of the NAC, transition energy, and dephasing time were more complicated in the case of cuboctahedral NPs. The smaller NAC of the (TiO₂)₉₇ rationalized its longer relaxation time compared to the (TiO₂)₂₉, but the presence of a singly coordinated oxygen atom greatly reduced the average transition energy, thus leading to a shorter relaxation time compared to (TiO₂)₇₈. Our results provide understanding on the effects of size and shape on the charge carrier dynamics in TiO₂ NPs, separating these effects from other factors, such as presence of defects, dopants, and adsorbates.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

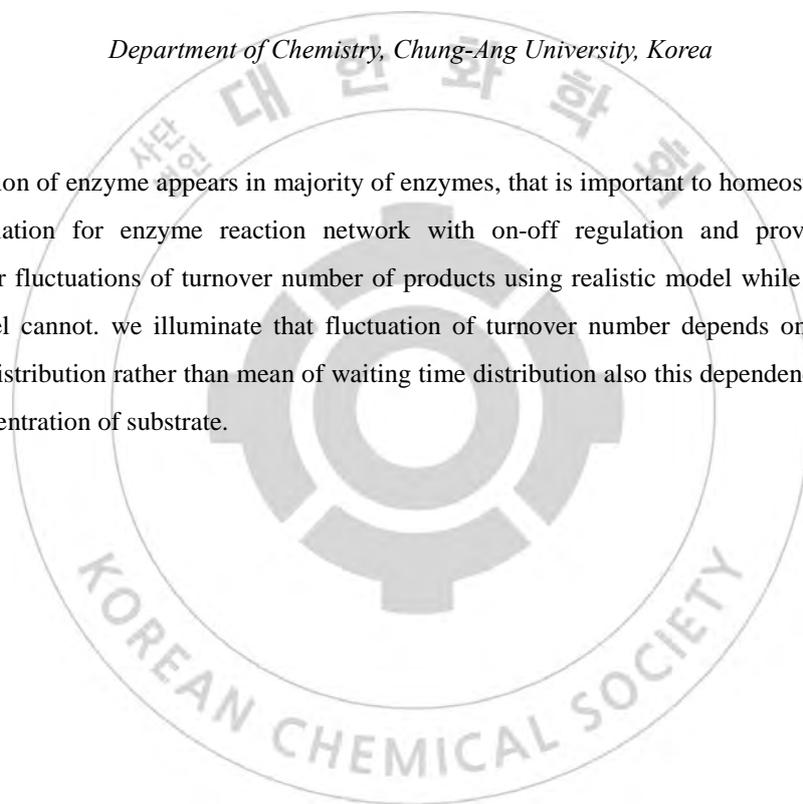
Exhibition Hall 2, FRI 11:00~12:30

Non-classical enzyme kinetics with on-off regulation

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Department of Chemistry, Chung-Ang University, Korea

On-off regulation of enzyme appears in majority of enzymes, that is important to homeostasis of cells. we conduct simulation for enzyme reaction network with on-off regulation and provide quantitative explanation for fluctuations of turnover number of products using realistic model while MM(Michaelis-Menten) model cannot. we illuminate that fluctuation of turnover number depends on randomness of waiting time distribution rather than mean of waiting time distribution also this dependency of fluctuation varies by concentration of substrate.



Poster Presentation : **PHYS.P-194**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Study on the effect of the hydrophobic interaction between lipid molecules on the lipid flip-flop motion in lipid vesicles

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Department of Chemistry, Hannam University, Korea

In this study, we prepared model membranes in order to understand biophysical behavior of the lipid molecules in biomembranes. Large unilamellar vesicles (LUV) were prepared with different ratios of two 1,2-Dimyristoyl-sn-glycero-3-phosphocholines (DMPC) and 1,2-diheptanoyl-sn-glycero-3-phosphocholines (DHPC) each of which has a different hydrophobic length. The contribution of the hydrophobic interaction to the total interactions between lipids was investigated by measuring the flip-flop rate of lipid molecules in LUV. To measure the flip-flop rates of lipid molecules in LUV, 1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine-N-(7-nitro-2-1,3-benzoxadiazol-4-yl) ammonium salt (NBD-PE) was incorporated into the [DMPC+DHPC] LUVs. The flip-flop rates were calculated by the fluorescence intensity changes of NBD-PE with time by quenching the fluorophore NBD-PE with sodium dithionite. The experiments were performed in the range of 25 °C ~ 45 °C and the activation energies at the different ratios of DMPC and DHPC were calculated from the experimental data. Activation energies for the flip-flop of NBD-PE molecule were 58 kJ/mol and 84 kJ/mol in DMPC LUVs and in [DMPC:DHPC=3:1] LUVs, respectively. This means that the activation energy increases by 14 kJ/mol when a DMPC molecule among six lipid molecules surrounding NBD-PE molecule is replaced with a DHPC molecule.

Poster Presentation : **PHYS.P-195**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Theoretical Study on Chemical Reaction Mechanisms of 1,3-C₄F₆

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Hexafluoro-1,3-butadiene (1,3-C₄F₆), having much lower global warming potential (GWP) value and atmospheric lifetime than c-C₄F₈, is used in selective etching processes of silicon oxide (SiO₂) on Si and silicon nitride (Si₃N₄) layers of fabricating contact holes in ultralarge integrated circuits.[1,2] In this work, the transition structures and activation energies on the gas-phase isomerization and dissociation paths of 1,3-C₄F₆ were calculated at the DFT(wB97X-D/avtz) level and compared with ones of c-C₄F₈. It is expected that our theoretical results give us the useful information about the CF₂, CF₃, C₃F₃, and C₃F₄ formation mechanisms of 1,3-C₄F₆ in plasma phases. References:[1] M. Nakamura et al., J. Vac. Sci. Technol., 19, 2134 (2001)[2] R. Chatterjee et al., J. Electrochem. Soc., 149, G276 (2002)

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spectroscopic evidence of charge carrier transfer in aggregated DPAT-An nanocomposite

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The photophysical properties of organic molecule materials is directly linked to the charge transfer (CT) character. Various model systems have been studied to elucidate the CT dynamics. Donor- π -acceptor (D- π -A) conjugated system is a good model system for understanding charge transfer dynamics. We synthesized a new D- π -A conjugated system, DPAT-An, in which donor and acceptor are diphenylamine and diphenyl triazine, respectively. Donor and acceptor are linked with anthracene. Aggregated composite of DPAT-An accompanied the emission amplification. We applied the steady-state absorption and emission, and broadband transient absorption (TA) spectroscopy to unravel the behavior of excited charge carrier dynamics of this system in terms of the electronic structure. Here, we observed clear spectral change between DPAT-An monomer and the aggregated composite in solution. This can originate from the excited state characteristic of single quantum object.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Investigation of the triplet-triplet energy transfer mechanism between two cyclometalated iridium(III) complexes

Jin-Hyoung Kim, Changhyun Back, Su-Jin Kwak, Chul Hoon Kim*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In this study, we prepared phenylimidazole-based C^N-cyclometalated Ir(III) complexes (**DMP**, **TPF2**) and C^C-cyclometalated Ir(III) complex (**PMP**) and investigated the energy transfer process through intermolecular interactions between the two cyclometalated Ir(III) complexes. In films doped with 3% Ir(C^C)₃ complex (**PMP**) and 15% Ir(C^N)₃ complex (**DMP** or **TPF2**), the **PMP** effectively induced energy transfer to the **DMP** or **TPF2**. This intermolecular energy transfer process was investigated using a picosecond time-resolved emission spectroscopic method. One case of mixing **PMP** with **DMP**, two types of luminescence were observed at 470 nm and 580 nm, 470 nm was the emission due to **DMP**, while the emission at 580 nm can be assigned as the intermolecular exciplex emission. The other case of mixing **PMP** with **TPF2**, the emission at 465 nm corresponding to the **PMP** emission region decreased for 4.5 ns while the emission at 530 nm corresponding to **TPF2** increases. This emission can be assigned by energy transfer from **PMP** to **TPF2**. In addition, no change was observed in the longer wavelength region than the **TPF2** emission region for 10 μs. We analyzed the energy transfer process when **PMP** was added to the dopant (**TPF2**, **DMP**) and confirmed that **TPF2** was more efficient than **DMP**. Finally, it was confirmed that the operation lifetime and efficiency of the device were improved by doping 3% of **PMP** in EML.

Poster Presentation : **PHYS.P-198**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Influences of Bulky Substituent on the Phosphorescence Properties of Homoleptic Iridium(III) Complexes

Jin-Hyoung Kim, Su-Won Na, Min Su Choe, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A new series of homoleptic cyclometalated iridium(III) complexes based on the phenylpyridine (ppy) ligand containing bulky substituents have been synthesized and characterized. The phosphorescence behavior of Ir complexes is investigated by steady-state and time-resolved emission spectroscopic techniques. Comparison of the results with those of the reference **Ir(ppy)₃** reveal that the emission color and photophysical properties of the other Ir complexes are influenced by the electron-donating groups (-CH₃ and phenyl derivatives) attached to the ppy ligand. In particular, systematic red-shifts are observed by increasing the electron-donating ability. The emission spectrum of **Ir(Me-ppy)₃**, having small electron-donating -CH₃ group, is red-shifted; however, the emission quantum yield is low and the nonradiative decay constant is large. On the other hand, although bulky phenyl derivative-adducts (**Ir(Ph-ppy)₃**, **Ir(MePhppy)₃**, and **Ir(diMePh-ppy)₃**) also exhibit red-shifted emission, but their kinetic and photophysical behaviors are more optimal than those of **Ir(Me-ppy)₃**, whose behavior does not follow the energy gap law. This deviation may be attributed to the rigid environment associated with the steric hindrance of a bulky substituent. The molecular structure, molecular orbitals in singlet/triplet manifolds, and energy band gap are verified by density functional theory calculations.

Poster Presentation : **PHYS.P-199**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The existence of protonated oxygen with iodide ion and its role in the formation of triiodide ion

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Department of Chemistry, Kyungpook National University, Korea

The presence of gaseous iodine in the polar and marine boundary layers is of great interest because this highly reactive species can affect the oxidative capacity of Earth's atmosphere. The abiotic photo-oxidation mechanism of I⁻ to I₃ and I₂ in the ice phase was suggested in previous study. To understand mechanism, The CASSCF(7,12) was employed for (I⁻·O₂) complex in gas phase. However, we found gas phase (I⁻·O₂) complex mechanism not enough to explain experimental result. So, we derive the acidic condition on system by adding proton on (I⁻·O₂) complex. The IO₂H complex shows the key step of mechanism which charge transfer from iodide to oxygen molecule. The role of light also investigated with time-dependent density functional theory.

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The Intraband Transition of Less Toxic Self-Doped Metal Chalcogenide Nanocrystal

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¹*Department of Chemistry, Korea University, Korea*

For decades, colloidal quantum dots have been in the spotlight as optical materials due to the tunable band gap transition. Due to the quantum confinement effect, continuous states within the band are confined to discrete states. Intraband transition occurring between discrete states of the semiconductor nanocrystal, in principle, should allow many applications in various fields because of their small energy. However, due to the fast hot electron relaxation, it had been very difficult to use the intraband transition. In 2014, the steady-state intraband transition in the mid-IR was first reported by Jeong et al. This is a novel result that opens up the possibilities for using the new electron transition of the colloidal semiconductor nanocrystals, particularly in the mid-IR region. Despite the incredible results, there was a concern in dealing with a toxic reagent such as mercury ion compounds. Thus, there has been a demand for replacement with less-toxic materials. In this poster, I will present the optical properties of silver selenide colloidal quantum dots(CQDs) showing the steady-state intraband transition in the mid-IR. In previous studies, Sahu et al. reported that silver selenide CQDs having absorption around 2000 cm⁻¹, but they incorrectly interpreted it as the band gap transition. Based on our own spectroelectrochemistry and mid-IR emission spectroscopy results, we proved that the mid-IR electronic transition of the silver selenide CQDs arises from the intraband transition. The silver chalcogenides relatively less toxic material will enable many researchers to access to the steady-state intraband transition of the colloidal quantum dot study.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Assessment of the MR-SF-TDDFT for conical intersections

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The conical intersections (CIs) are established to be very important points on the potential energy surface (PES). According to its definition, CI corresponds to a set of molecular geometries where PESs of two electronic states are degenerate. They play an important role in the field of photochemistry serving as a source of non-adiabatic transitions between two PESs. Recently developed in our group, mixed-reference spin-flip time-dependent density functional theory (MR-SF-TDDFT) has been tested for its ability to precisely describe CI structures in series of organic molecules. For these calculations, BHHLYP DFT hybrid functional has been employed along with 6-31+G* basis set. The results obtained here have been compared with those from previous calculations, i.e., ab initio multireference configuration interaction with single and double excitations (MRCISD), state-interaction state-averaged restricted ensemble-referenced Kohn-Sham method (SSR), and spin-flip time-dependent density functional theory (SF-TDDFT). As shown, the new method is able to describe CI geometries precisely. Root-mean-square deviation values between MR-SF-TDDFT and other methods do not exceed 0.21 Å. The analysis of branching plane vectors has been carried out for all the molecules with the aim to confirm the correct dimensionality of CI seam. Our results support the use of MR-SF-TDDFT for the accurate CI description.

Poster Presentation : **PHYS.P-202**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Origin of high reactivity and enhanced endo/exo selectivity in water-accelerated Diels-Alder reactions

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The Diels-Alder reaction is a very powerful method widely used in organic synthesis since it allows one to form two C–C bonds in one step. Some Diels-Alder reactions that were believed for a long time to be almost insensitive to solvent choice are accelerated in water as well as their endo/exo selectivity is enhanced [1]. Previous theoretical calculations made an attempt to elucidate this high reactivity in terms of hydrogen bond formation between solvent molecules and a polarized transition state (TS). However, an explanation regarding enhanced endo/exo selectivity is still missing. Here, ab initio static calculations as well as molecular dynamics simulations were performed for the Diels-Alder reaction between C₅H₆ (cyclopentadiene) and two dienophiles, i.e., CH₂=CHCN and CH₂=CHCHO to clarify the origin of the high reactivity and to understand the reason for the enhanced endo/exo selectivity in water. The simulations were done in polar H₂O solvent and in less polar CH₂Cl₂. As shown, solvent molecules cause charge polarization of TS, in particular, the polarization of the –CN and –CHO groups. H₂O gives rise to stronger effect in comparison with CH₂Cl₂. The TS structure is not rigid as thought before, but flexible with a wide distribution of one out of two forming C–C bonds. Moreover, a bifurcation point that may affect endo/exo selectivity was found to lie earlier than the TS point on the free energy surface. Also, a particular orientation of the dienophiles with respect to the diene was found in a reactant region. This is attributed to dipole-dipole interactions. These and other results are further discussed.[1]. D. C. Rideout, R. Breslow J. Am. Chem. Soc. 1980, 102, 7816.

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Formation of Fe(III)-Oxyl Species in the C-H Activation by Non-Heme Iron-Oxo Complexes : DFT Studies.

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High valent iron-oxo compounds have been proposed to play an important role in the catalytic cycle of alkane hydroxylation. Extensive studies have been conducted to identify the alkane hydroxylation mechanism of non-heme iron-oxo complexes. The formation of Fe(III)-oxyl species during the reaction to abstract hydrogen atom from alkane has been proposed, however this proposal has yet been reached a consensus. To identify the formation of Fe(III)-oxyl species during the reaction, we monitored the change of Hirschfeld spin density along the reaction coordinates of hydrogen abstraction by two non-heme iron-oxo complexes, $[\text{FeO}(\text{H}_2\text{O})_5]^{2+}$, and $[\text{FeO}(\text{H}_2\text{O})_4(\text{NH}_3)_2]^{2+}$. By calculating minimum energy paths of two complexes, and analyzing donor-acceptor interactions of natural bond orbitals along the minimum energy paths, this study revealed that Fe(III)-oxyl species are formed only in the C-H activation of high spin non-heme iron-oxo complexes and lowers the activation energy.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

CTAB-modified AuNPs for sensitive SERS measurement

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Gold nanoparticles (AuNP) are widely used in many applications including nanosensors for delivering chemical information in biological system. AuNPs are generally considered inert, nontoxic, and thus biocompatible, but the efficient surface adsorption on AuNPs is possible for molecules with a limited functional groups including carboxyl and thiol groups. Thus the surface modification of AuNPs for facile attachments of analytes onto AuNP is indispensable for the sensitive detection by SERS. In this research, a simple method of surface modification of citrate-reduced AuNPs by cetyl trimethylammonium bromide (CTAB) is introduced. SERS of hydroxyanthraquinones were greatly enhanced with the CTAB modified AuNP, where the efficient aggregation of AuNP occurs due to less negative surface charges of CTAB modified AuNP. SERS of 1,2-dihydroxyanthraquinone (alizarin) in either neutral or deprotonated form on the CTAB modified AuNP was obtained. Polyaromatic hydrocarbons (PAHs) generated in pyrolysis or incomplete combustion, and easily accumulated in soil or water in particulate matter. PAHs not readily biodegradable and often accumulated in organisms are generally known as immunosuppressant or carcinogen. We show that SERS detection of PAHs by CTAB modified AuNP can be used as an efficient analytical tool with high reproducibility and selectivity. A simple protocol for the detection and identification of various PAHs based on the Raman spectra will be introduced.

Poster Presentation : **PHYS.P-205**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

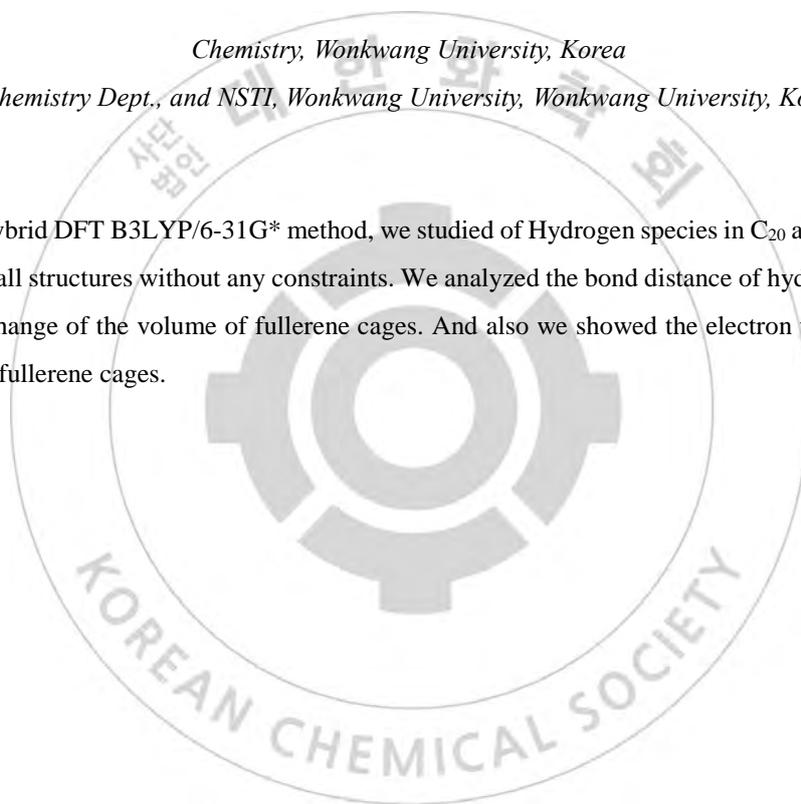
Study of Hydrogen species in C₂₀ and C₇₀ Fullerenes

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By using the hybrid DFT B3LYP/6-31G* method, we studied of Hydrogen species in C₂₀ and C₇₀ fullerene. We optimized all structures without any constraints. We analyzed the bond distance of hydrogen species in cage and the change of the volume of fullerene cages. And also we showed the electron transfer between Hydrogen and fullerene cages.



Poster Presentation : **PHYS.P-206**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Understanding the Electrochemical Reaction in the Polybromide Battery System

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Polyhalide species have been used in wide range of applications such as halogenation reactions, nanomaterial modification, and so on. Even though most of studies for polyhalide have been performed based on iodine, polyhalide species consisting of bromine have recently had an attraction due to their lower atomic mass in comparison with iodine. It indicates that polybromide species have higher energy density than polyiodide species when they are playing a role as an energy material. Hence, polybromide species have been received a great attention as an electrochemical energy storage (EES) material. In this study, we have been trying to prepare a novel type of battery system, polybromide battery (PBB), using polybromide species as an energy generation/storage material. Based on the initial discharging potential of PBB and the equilibrium reaction of bromine species in the aqueous media, we suggests that the reduction of bromine species in the polybromide is not a primary reaction on the electrode but an indirect reaction. After discharging tests for various polybromide species, we obtained Raman spectra of polybromide remained in the PBB system in order to investigate the variation in the main species of polybromide. The resulting Raman spectra were found that bromine weakly bound to the complexing agent in polybromide species is initially reacted on the carbon electrode in discharging reaction and the bromine strongly bound was not participated on the discharging reaction. Our results aid to understanding the mechanism of charging/discharging reactions of the PBB system.

Poster Presentation : **PHYS.P-207**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Strange Cargo Delivery Dynamics in Living Cells

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Vesicle-transport conducted by motor-protein-multiplexes, ubiquitous among eukaryotes, shows mysterious stochastic dynamics, qualitatively different from dynamics of thermal motion and artificial active matter; the relationship between in vivo vesicle-delivery dynamics and dynamics of the underlying physicochemical processes is not yet quantitatively understood. Addressing this issue, we perform accurate, label-free tracking of individual vesicles, containing probes free of photobleaching or photoblinking, transported by kinesin-dynein-multiplexes along axonal microtubules in human neuroblastoma cells. The mean-square-displacement of vesicles along the microtubule exhibits unusual dynamic phase transitions, seemingly inconsistent with the scaling behavior of the mean-first-passage time over the travel length. These paradoxical results and the vesicle displacement distribution at all times are quantitatively explained and predicted by a multi-mode motor multiplex model where ATP-hydrolysis-coupled motion of kinesin-dynein-multiplexes has both unidirectional and bidirectional modes. This work presents a new paradigm of quantitative biology, ushering in a new age of quantitatively understanding and predicting mysterious biological phenomena through the analytical power of mathematical deduction informed by physics and chemistry.

Poster Presentation : **PHYS.P-208**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Histidine ($\delta\delta\delta$) and ($\epsilon\epsilon\epsilon$) tautomer effect on early oligomerization stage of the amyloid-beta peptide (1-40)

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As one of the main types of dementia, the Alzheimer disease (AD) is connected to the accumulation of amyloid-beta peptide ($A\beta$) in the brain. Important factors such as amyloid concentration, pH, solvent, histidine behavior and metal ions can affect the aggregation progress. $A\beta$ oligomer hypothesis and experimental results have shown the higher toxicity of small oligomers (dimers, trimers, etc.) compare with fibrils which indicates the importance of investigation of aggregation at the early stages in details. Since many aspects at this level is still unknown so here molecular dynamic (MD) simulation of $A\beta(1-40)$ homodimers considering the ($\delta\delta\delta$) and ($\epsilon\epsilon\epsilon$) tautomeric effects with different initial conformations were performed using GROMACS 5.0 software to elucidate structure changes during aggregation. Results showed very low propensity or almost no tendency to form β -sheet for ($\epsilon\epsilon\epsilon$) homodimers. However in ($\delta\delta\delta$) homodimers higher content of β -sheet during aggregation can be observed which may show the higher neurotoxicity. Also β -sheet formation in ($\delta\delta\delta$) dimers can be found in almost same regions (CHC and C-/N- terminal). Our study may provide better understanding of tautomeric behavior of histidine on $A\beta(1-40)$ aggregation and disease progression which may lead to find some ways to cure the AD.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Particle Size-Dependent Metal-Enhanced Fluorescence of Dyes on Homogeneous Silver Colloidal Surfaces

Daedu Lee, Junghyun Song, Yoonsoo Pang*

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

Metal-enhanced fluorescence (MEF) has been extensively studied in many disciplines due to significant increases in the emission intensity and photostability of dyes. In this study, homogeneous silver colloidal films (SCFs) with the particle diameters from ~70 to 200 nm were fabricated for fluorescence enhancements. MEF and excited state dynamics of DCM and Rh700 with SCFs were investigated by time-resolved fluorescence spectroscopy, where fluorescence enhancements were stronger where the dipolar SPR bands of SCFs overlap with the emission spectra of dyes. Although the particle size-dependence of fluorescence enhancements with SCFs mainly arises from the excitation enhancements, the emission enhancements of dyes with small quantum yields are often overestimated with an assumption of $k_{nr,m} \approx k_{nr}$. We propose an improved analysis method, which is based on the fluorescence enhancements with a SCF in off-resonance with the emission bands of dyes, and the FDTD simulations for the average local electric fields. By this method, the particle size-dependent excitation and emission enhancements of Rh700 with all SCFs were precisely evaluated. The MEF of Rh700 with SCFs is mainly attributed to the excitation enhancements, but also shows a strong particle size-dependence.

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Time-resolved Structural Dynamics of para-Halogen-disubstituted trans-Stilbene

Dong-gu Kang, Chan Ho Park¹, David W. McCamant², Sang Kyu Kim*

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

²*Department of Chemistry, University of Rochester, United States*

We have studied the photoisomerization reaction of 4,4'-dichloro-trans-stilbene (44DchtS) and 4,4'-dibromo-trans-stilbene (44DBrtS) in the condensed-phase with femtosecond transient absorption and femtosecond stimulated Raman spectroscopy. Coherent oscillation features were observed in the excited-state absorption signal and the frequencies of the coherent motion showing the in-plane bending mode at 150 cm^{-1} (44DchtS) and 120 cm^{-1} (44DBrtS) are induced by para-halogen-disubstituent. In n-hexane (acetonitrile), photoisomerization lifetime of 44DchtS and 44DBrtS are 314 (124) ps and 85 (65) ps, respectively. In the case of 44DBrtS, we expect another C-Br bond dissociation reaction pathway since TD-DFT calculation shows the low dissociation barrier of C-Br coordinate compared to that of C-Cl. Also, we observed that the C=C stretching mode of transient Raman spectra (1550 cm^{-1}) depends on the excess energy of excitation pulse. Therefore, we will present the time-resolved structural dynamics of S_1 state in 44DchtS and 44DBrtS comparing the substituent effect to that of trans-stilbene.

Poster Presentation : **PHYS.P-211**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Twisted intramolecular charge transfer state of push-pull emitters investigated by time-resolved Raman spectroscopy

Sebok Lee, Myungsam Jen, Yoonsoo Pang*

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

Intramolecular charge transfer (ICT) process, one of the fundamental chemical reactions, has been widely investigated for many decades. Since the ICT process is initiated by charge separation from the electron donor to the acceptor, the structural changes of molecules upon photoexcitation may hold the important key to the reaction mechanisms. In this work, the twisted ICT states of “push-pull” emitters, DCM and LD 688, were explored by femtosecond stimulated Raman spectroscopy. The ICT process of ~1 ps was followed by the vibrational relaxation of ~5 ps, which is monitored by $\delta(\text{CH}/\text{CH}_3, 1200 \text{ cm}^{-1})$, $\nu(\text{C}=\text{C}, 1475 \text{ cm}^{-1})$, $\nu(\text{C}\equiv\text{N}, 2170 \text{ cm}^{-1})$. A twisted geometry with rotated dimethylamino or dimethylaminophenyl group was proposed based on the TDDFT simulations. The ICT dynamics of 4-dimethylamino-4'-nitrostilbene dye was also studied, where the rotation of nitrobenzene group was clearly evidenced by the spectral changes of $\nu(\text{C}=\text{C}, \text{ring})$ mode at 1600 cm^{-1} . A time-resolved impulsive stimulated Raman setup currently in construction will also be introduced, where the frequency-domain vibrational spectra were obtained by fast Fourier transformation of the temporal coherent nuclear wavepacket motions which are impulsively excited by ultrashort Raman pump. With the impulsive Raman probe, the structural changes during the ICT process of the push-pull emitters, especially in the low frequency region of $^{-1}$, will further be explored.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

In-Silico Screening of Iron(IV)-Oxo Complexes as C-H Bond Activation Catalysts Using Machine Learning Algorithms

Jiwoo Choi, Yongho Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Developing catalysts for C-H activation was one of the long-standing concerns of transition metal chemistry. Therefore, many studies on the Fe(IV)-oxo complexes as a model of active species in P450 or TauD have been carried out, but no optimal catalyst has yet been made for practical use. In developing a new catalyst, DFT calculations have successfully been used to predict the structure and explain catalytic properties. Therefore, in-silico screening in advance by using machine learning techniques can be used as a powerful tool to develop a new catalyst. In this study, we made a database of Fe(IV)-oxo compounds with heme and non-heme ligands (both in the high and low spin states) to train and test machine learning. Various parameters in relation to the catalytic activity were modeled and learned by using machine learning algorithms. We will present a machine-learning models to predict the activation energy of the catalyst quickly and accurately without extensive DFT calculations.

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

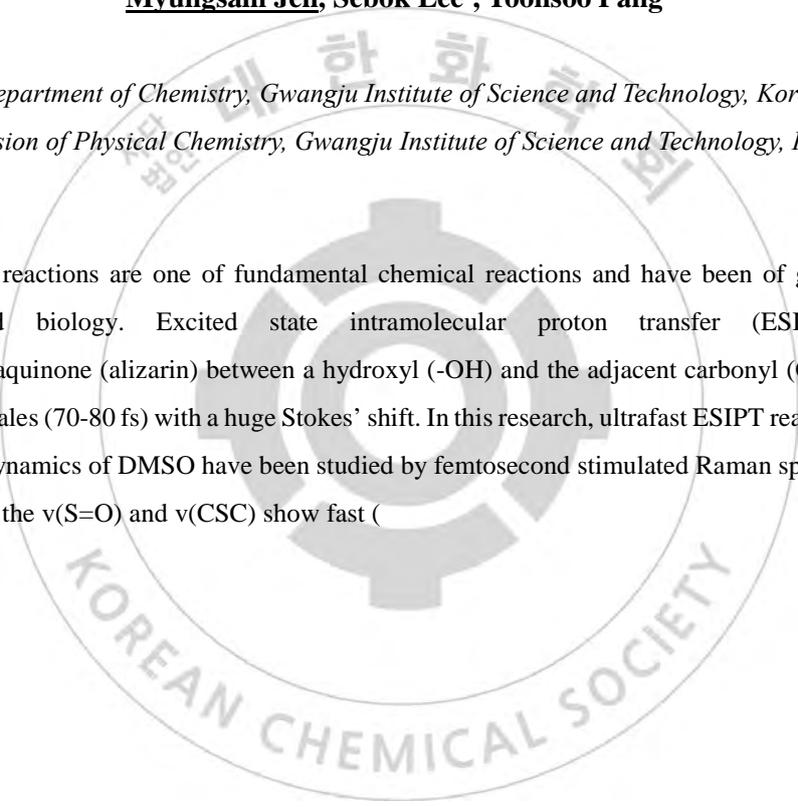
Intramolecular proton transfer reactions strongly coupled to the solvation dynamics of DMSO

Myungsam Jen, Sebok Lee¹, Yoonsoo Pang*

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

¹Division of Physical Chemistry, Gwangju Institute of Science and Technology, Korea

Proton transfer reactions are one of fundamental chemical reactions and have been of great interest in chemistry and biology. Excited state intramolecular proton transfer (ESIPT) of 1,2-dihydroxyanthraquinone (alizarin) between a hydroxyl (-OH) and the adjacent carbonyl (C=O) occurs on ultrafast time scales (70-80 fs) with a huge Stokes' shift. In this research, ultrafast ESIPT reaction of alizarin and solvation dynamics of DMSO have been studied by femtosecond stimulated Raman spectroscopy. We have found that the $\nu(\text{S}=\text{O})$ and $\nu(\text{CSC})$ show fast (



Poster Presentation : **PHYS.P-214**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Quantitative study of mammalian gene expression based on transcriptional interactome model

Jaehyuk Won, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

In mammalian cells, actively transcribed genes are organized to be in close proximity to each other, forming transcriptional interactome. For genes belonging to an interactome, their expressions are highly correlated in a positive sense. In addition, it has been recently found that transient or stable aggregates of RNA polymerase (RNAP) II molecules are formed around such interactomes. Understanding how mammalian gene expression is influenced by such factors is still missing. In order to provide an analytical framework targeting this problem, we present the mammalian gene expression model with RNAP II cluster dynamics and gene activity fluctuation taken into account. From the RNA-sequence experimental data over five human breast cancer cell lines, we could extract the correlation-noise relationship for genes transcribed through basal promoters and multi-gene interactomes. It is shown that the present theory can make a quantitative prediction to the experimental result in conjunction with three different degradation models

Poster Presentation : **PHYS.P-215**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

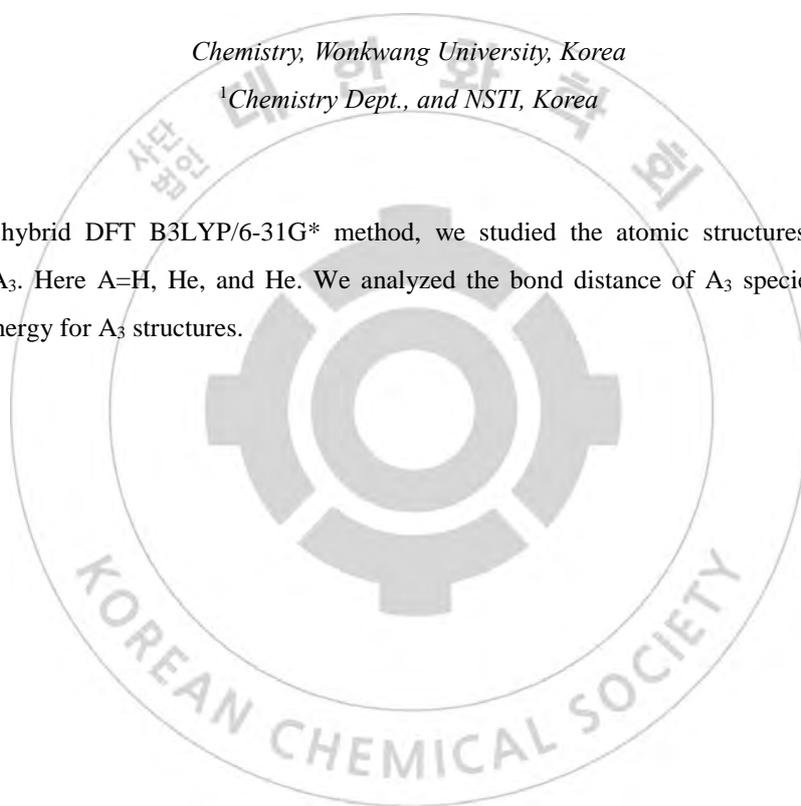
Atomic Structure and Electronic Properties of A_3 (A=H, He, and He)

Han-Su Hwang, Kee Hag. Lee^{1,*}

Chemistry, Wonkwang University, Korea

¹*Chemistry Dept., and NSTI, Korea*

By using the hybrid DFT B3LYP/6-31G* method, we studied the atomic structures and electronic properties of A_3 . Here A=H, He, and He. We analyzed the bond distance of A_3 species. And also we analyzed the energy for A_3 structures.



Poster Presentation : **PHYS.P-216**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photophysical property calculation of cycloparaphenylene(CPP) and carbon nanobelt(CNB) using long-range corrected DFT

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As a starting point of our application and assessments of theoretical methods to photophysical of carbon nanotube systems, we performed Time-Dependent Density Functional Theory(TD-DFT) calculations using Long-range Corrected(LC) DFT and conventional B3LYP functionals to investigate whether the DFT calculation can reproduce the UV-visible adsorption spectrum of cycloparaphenylene(CPP) and carbon nanobelt(CNB)[1,2]. Experimental spectrum for 12-CNB shows that the maximum absorption wavelength is 313nm. (Figure 1) However, the maximum absorption wavelength of B3LYP spectrum is 333nm, those of LC-BOP changed in range separation parameter μ and LCgau-B97 are 302nm and 305nm, which shows that LC-BOP and LCgau-B97 successfully reproduced the experimental spectra while B3LYP overestimated the experimental spectra. Furthermore, B3LYP spectrum has weak absorption at 421nm while LC-BOP and LCgau-B97 have it at 340nm which consistent with weak absorption wavelength(near 350nm) of experimental spectra. References :[1] Povie, G. Segawa, Y. Nishihara, T. Miyauchi, Y. Itami, K. J. Am. Chem. Soc, 2018, 140(31), 10054[2] Iwamoto, T. Watanabe, Y. Sakamoto, Y. Suzuki, T. Yamago, S. J. Am. Chem. Soc. 2011, 133, 21, 8354

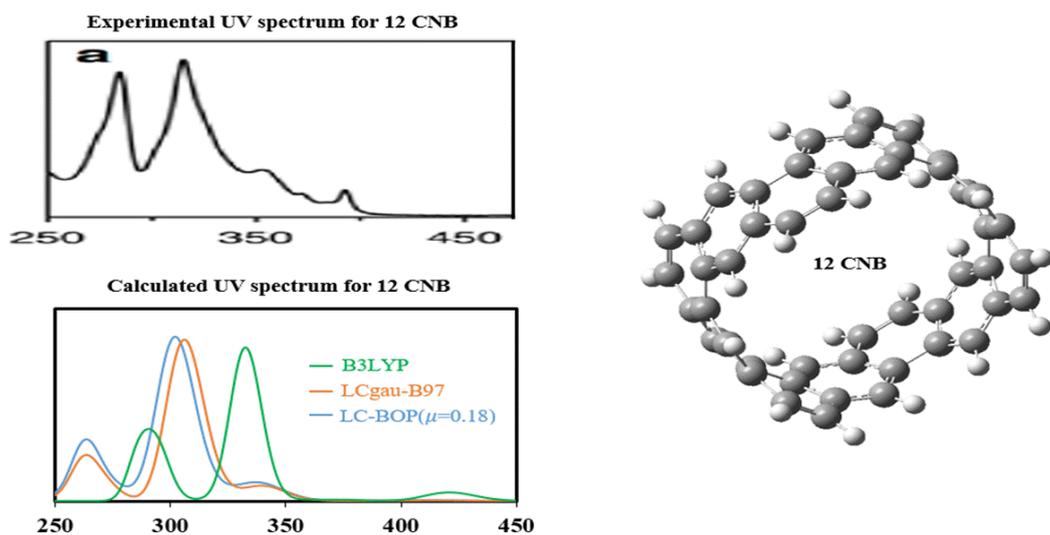


Figure 1. Experimental and calculated UV spectrum for 12 CNB and 12-CN structure



Poster Presentation : **PHYS.P-217**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Reproduction of Experimental UV/Vis Absorption spectrum of Pyrene Excimer using Long-range Corrected DFT Calculation

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We investigate the ultraviolet visible absorption spectrum of syn- and anti-pyrene using various exchange functional of density functional theory to time-dependent (Td) density functional theory(1). We showed that the Long-range Corrected density functional LCgaub97 accurately reproduced the experimental ultraviolet visible absorption spectrum. But the B3LYP and other functionals under- or over-estimated the experimental spectra. The poor TDDFT results for pure functionals may be due to lack of long-range orbital-orbital interactions. We also investigate the effect of solvents with various functionals.

References:1(a)

- Song,J.W.;Hirao,K.J.Chem.Phys.2015,143(14),144112;(b)Song,J.W;Hirao,K.J.Comput.Chem.2011,32(15)(c) Song,J.W;Hirao,K.J.Theor.Chem.Acc.2013,133(2);
(d)Tawada,Y.;Tsuneda,T.;Yanagisawa,S.;Yanai,T.;Hirao,K.J.Chem.Phys.2004,8425-33.2.(e)H.Likura,T.Tsuneda,T.Yanai,andK.Hirao,J.Chem.Phys.115,3540(2001).3.(f)J.W.Song,T.Hirosawa,T.Tsuneda,and K.Hirao,J.Chem.Phys.126,154105(2007).

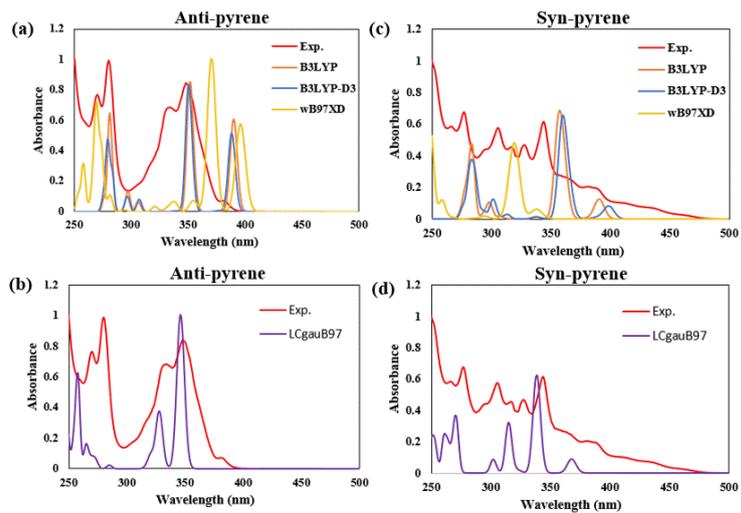


Figure 1. Calculated and experimental UV-Vis spectrum of anti-pyrene(a,b) and syn-pyrene(c,d) with various DFT functional at TD /6-311++g(d,p) level of theory



Poster Presentation : **PHYS.P-218**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photodissociation dynamics of methyl mercaptan (CH_3SH) in gas phase

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Photodissociation of methyl mercaptan, known as the simplest alkyl thiol, has been reported. A major issue of previous studies was a coupling of two excited potential energy surfaces (PES) $1A''$ and $2A''$ depending on the wavelengths of photo-excitations. H atom followed by photoexcitation of 193, 248 nm had been studied using high Rydberg n time of flight method [1]. Ion imaging experiment using ~243.1 nm was also employed [2]. The $1A''/2A''$ conical intersection points were calculated using over a 1 million configuration state function [3]. Although $\cdot\text{CH}_3$ velocity map imaging (VMI) using 204 nm pump and different probes had been studied, the corresponding H VMI had not been reported yet [4,5].

Here, we obtained H VMI using one color ~243.1 nm wavelength. Compared to the previous work, we observed vibrational progressions for the methylthio radical ($\text{CH}_3\text{S}\cdot$). S-C stretching and CH_3 umbrella motion could be assigned as those progressions qualitatively. Experiments using doppler reduced method and infrared laser beam (IR-UV double resonance) are in progress. We expect that IR-UV vibrationally mediated photodissociation would give clues for the way of passage of $1A''/2A''$ conical intersection in the excited state molecule.

- [1] J. Chem. Phys. 1993, 99 (9), 6600
- [2] J. Chem. Soc., Faraday Trans., 1996, 92(24), 5181-5183
- [3] J. Chem. Phys., 1994, 100, 3639
- [4] Phys. Chem. Chem. Phys., 2011, 13, 8531-8536
- [5] J. Chem. Phys., 2007, 126, 024301

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characterization of Copper Nanoparticles Produced by Pulsed Laser Ablation in Liquids

Talshyn Begildayeva, Seung Jun Lee, Seung Heon Lee, Tae Ho Kim, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Herein, comparative experiments were carried out to identify the effect of various organic solvents on the composition and morphology of nanoparticles formed by pulsed laser ablation (PLA) of a solid copper target in liquids. Deionized water, acetonitrile, methanol, ethanol and hexane were used to obtain colloidal copper nanoparticles. We show nanoparticles with different morphology can be produced with using a simple and safe preparation method. Moreover, according to results of powder x-ray diffraction analysis, the species differ not only in shape, but also in composition, namely, when laser ablation of a solid copper target in acetonitrile is carried out along with copper metal nanoparticles with a core-shell structure (Cu@C), copper (I) cyanide micro sized particles are formed. While spherical particles of copper (I) and (II) oxide are formed in deionized water and alcohols methanol and ethanol, respectively. The latter, in turn, aggregates into larger rod-like particles. Size and morphology of the nanoparticles were confirmed by transmission electron microscopy, scanning electron microscopy and ultraviolet-visible spectrometry. Raman spectroscopy and powder x-ray diffraction technique were also used to characterize samples. We conclude that the ablation of copper plate in various liquid media is a facile method for producing of copper and copper-based nanoparticles without the use of any surfactants or precursors.

Poster Presentation : **PHYS.P-220**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of Ag@Lignin Hybrid nanocomposite using pulse laser irradiation

Seung Jun Lee, Seung Heon Lee, Talshyn Begildayeva, Juhyeon Park, Tae Ho Kim, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

In this study silver@lignin nanocomposites have been synthesized using pulse laser irradiation (PLI) techniques. Lignin is well-known biopolymer which is usually used as biosensors and catalysts. Making silver@lignin nanocomposite using PLI is new way for green chemistry. Nanocomposite with high efficient was synthesized by PLI technique using aqueous AgNO_3 as a precursor. In the method lignin used as a reducing agent as well as additive capping agent. The use of a laser generated catalyst, has been able to effectively decompose various chemical species such as methylene blue, p-nitrophenol and H_2O_2 .

Poster Presentation : **PHYS.P-221**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Comparative Study on the Binding Characteristics between α -helix Mimetic Small Molecule/MCL-1 Complexes

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Department of Chemistry, Sookmyung Women's University, Korea

Anti-apoptotic protein MCL-1 promote cellular survival by trapping the critical apoptosis-inducing BCL-2 homology domain 3 (BH3) α -helix of pro-apoptotic BCL-2 family members. Cancer cells exploit this physiologic survival mechanism through anti-apoptotic protein overexpression, establishing an apoptotic blockade that secures their immortality. Inhibition of interaction between the BH3 and MCL-1 is thus significant for suppressing the growth of cancer cells. Recently, scaffolds as α -helix mimetic small molecule such as various triazine-piperazine-triazine structures have been designed for binding affinity with MCL-1. Here, we report the structural and thermodynamic characteristics for the binding complexes of the α -helix mimetic small molecules to MCL-1. We performed molecular dynamics simulations to investigate the structural properties of the complexes. The binding free energy calculations based on the integral equation theory was then executed to quantify the binding affinity for the complexes and to understand the factors responsible for the binding affinity.

Poster Presentation : **PHYS.P-222**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Intramolecular Charge Transfer Dynamics of Dyes inside AOT Reverse Micelles

Gisang Lee, Taehyung Jang, Yoonsoo Pang*

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

Photo-induced intramolecular charge transfer (ICT) processes in dye molecules have been of great interest in biology and chemistry fields for 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. The torsional angle of 4-dimethylamino-4'-nitrobiphenyl (DNBP) between two phenyls is ~ 40 degrees in the ground state, but changes into planar or perpendicular geometry in the excited state depending on the solvent polarity. In this research, the excited state ICT dynamics of DNBP in the methanol/AOT/isooctane reverse micelles has been investigated by time-resolved fluorescence and transient absorption spectroscopy. We have observed strongly enhanced emission, the efficient intersystem crossing to the T1 state, and strong phosphorescence in the near-infrared region of DNBP in small reverse micelles, which is strongly related to the restricted torsional motion. In addition, excited state dynamics of similar push-pull dyes with internal degrees of freedom such as auramin O and thioflavin T have been investigated in the confined environment of reverse micelles.

Poster Presentation : **PHYS.P-223**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Frequency spectrum of Biological noise: A probe of non-classical reaction dynamics in living cells

Jingyu Kang, Ji-Hyun Kim^{1,*}, Jaeyoung Sung^{1,*}

Chemistry, Chung-Ang University, Korea

¹*Department of Chemistry, Chung-Ang University, Korea*

Contemporary chemical kinetics assume chemical reactions to be Poisson processes, reactions occurring in a single step. However, such assumptions are not realistically applicable to biological systems. In the living cells, reactions can occur quickly, starting and pausing, while other reactions consist of a number of steps. Such processes are known as non-Poisson processes. Here, for any independent birth-death process, we provide a general theory of the time correlation function (TCF) of product number fluctuation and the product number power spectrum (PNPS) for an arbitrary waiting time distribution of creation and degradation. This study not only shows that the PNPS contains more information of dynamics than the product noise but also sheds light on a general understanding of the effects non-Poisson creation and degradation processes have on the PNPS. For instance, we discover the general relationship between the relaxation time of the TCF and the relative variance of product creation time and product lifetime. Additionally, we reveal the general behavior of the PNPS in the large frequency limit. The correctness of our theory is verified using in-silico analysis. This study demonstrates that real-time counting of the product number is essential for a thorough analysis of reaction dynamics.

Poster Presentation : **PHYS.P-224**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

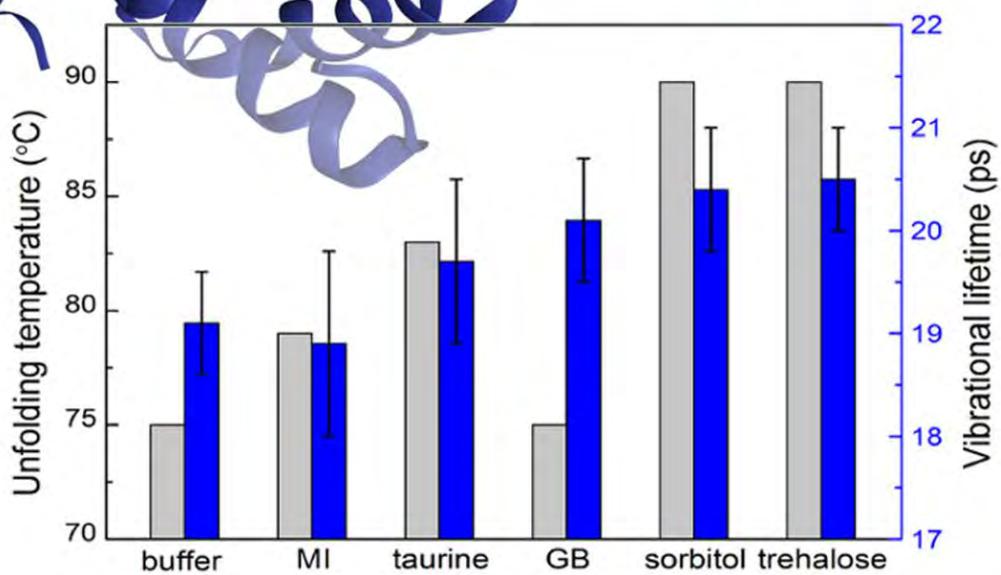
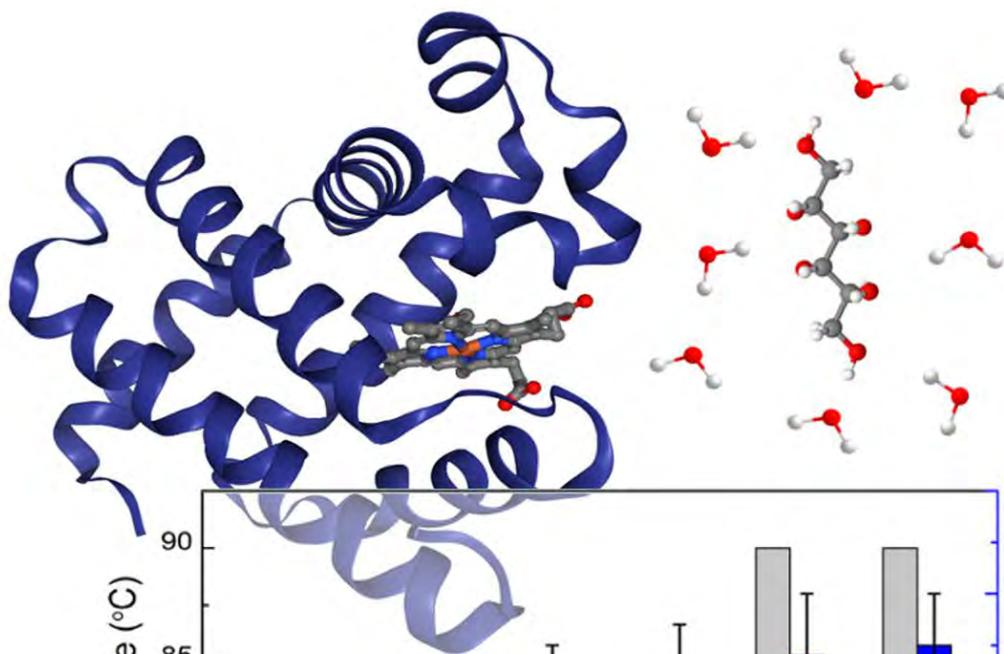
Do Osmolytes Impact the Structure and Dynamics of Myoglobin?

Dorota Kossowska, Kyungwon Kwak^{1,*}, Minhaeng Cho^{1,*}

Chemistry, Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

Osmolytes are small organic compounds that can affect the stability of proteins in living cells. The mechanism of osmolytes' protective effects on protein structure and dynamics has still not been fully explained. However, two possible mechanisms have been suggested and discussed - a direct interaction of osmolytes with proteins (water replacement hypothesis) and an indirect interaction (vitrification hypothesis). In order to investigate the effects of osmolytes on protein structure in an aqueous environment, we studied myoglobin-osmolyte systems using FTIR, UV-vis, CD, and femtosecond IR pump-probe spectroscopy. Interestingly, noticeable changes are observed in both the lifetime of the CO stretch of CO-bound myoglobin and the spectra of UV-vis, CD, and FTIR upon addition of the osmolytes. In addition, the temperature-dependent CD studies reveal that the protein's thermal stability depends on molecular structure, size of osmolytes and hydrogen-bonding ability. We believe that the present experimental results provide important clues about the complicated and intricate mechanism of osmolyte effects on protein structure and dynamics in a crowded cellular environment.



Poster Presentation : **PHYS.P-225**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Structural Colorations of Magnetoplasmonic Metamaterials for Colorimetric Sensing

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¹*Department of Cogno-Mechatronics Engineering, Pusan National University, Korea*

Controlling and understanding the assembly of colloidal nanoparticles remains a challenging issue for optimizing magnetic-plasmonic devices for various applications including sensors, displays, bio-imaging, and therapy. A magnetic field is successfully utilized to induce the fabrication of multidimensional structures composed of magnetoplasmonic (MagPlas) particles, which exhibit interesting optical properties. Notably, a magnetic-field assisted coating technique for fabrication of two-dimensional (2D) amorphous photonic crystal (APC) film of the MagPlas particles on a filter membrane is proposed. The MagPlas 2D APC exhibits strong dual reflected colors caused by structural scattering and plasmon resonance scattering. The water absorption ability of the membrane and the high refractive index sensitivity of plasmon resonance scattering are utilized to fabricate a simple colorimetric humidity sensor. Additionally, a mechanical colorimetric sensor that instantly exhibits responses to both bending and stretching forces is fabricated by embedding the 2D APC film into PDMS substrate. Because of unique features including dual-color characteristic, flexibility, and high plasmonic sensitivity, these kinds of the platform could be highly promising as wearable devices for physical, chemical and biological sensing with naked eye detection.

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Exploring the Role of Magnetoplasmonic Assembly in Electrochemical Oxygen Reduction Reactions

**Lemma Teshome Tufa, Van Tan Tran¹, Ki-Jae Jeong², Junyoung Kwon², Jeonghyo Kim²,
Jaebeom Lee^{1,*}**

Nano Fusion Technology, Ph.D. student at Pusan National University, Ethiopia

¹*Chemistry, Chungnam National University, Korea*

²*Department of Cogno-Mechatronics Engineering, Pusan National University, Korea*

The Lorentz or Kelvin force generated by externally applied magnetic field may introduce additional convection of electrolyte near working electrode and consequently caused magnetocurrent, which can be attributed to the magneto-hydrodynamic flows and extra electrochemical reaction. A composite of metallic and superparamagnetic nanoparticle is a promising candidate for such purpose from directional correlation to electromagnetic field. In particular, its 3-dimensionally (3D) ordered self-assembly may boost up the magneto-hydrodynamic flows on collectively reactive surfaces, leading to remarkable electrochemical performance. In this report, a proof-of-concept work explores the effect of magnetic field on electrocatalytic activity of reduction of oxygen. A precisely controlled 3D nanostructure of silver core-magnetic shell (Ag@Fe₃O₄) assembly was prepared and characterized. Then, the ratio of the reduction current of oxygen was carefully monitored in presence/absence of magnetic field. Computational simulation was also performed, in which the variance of magnetic field gradient force (Kelvin force) was calculated to prove the plausible mechanism from the assembled superparamagnetic nanostructure. From our experimental and computational fundamental research, it is probable that further effective electrocatalysts can be developed in the application of biomedical and energy industries.

Poster Presentation : **PHYS.P-227**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

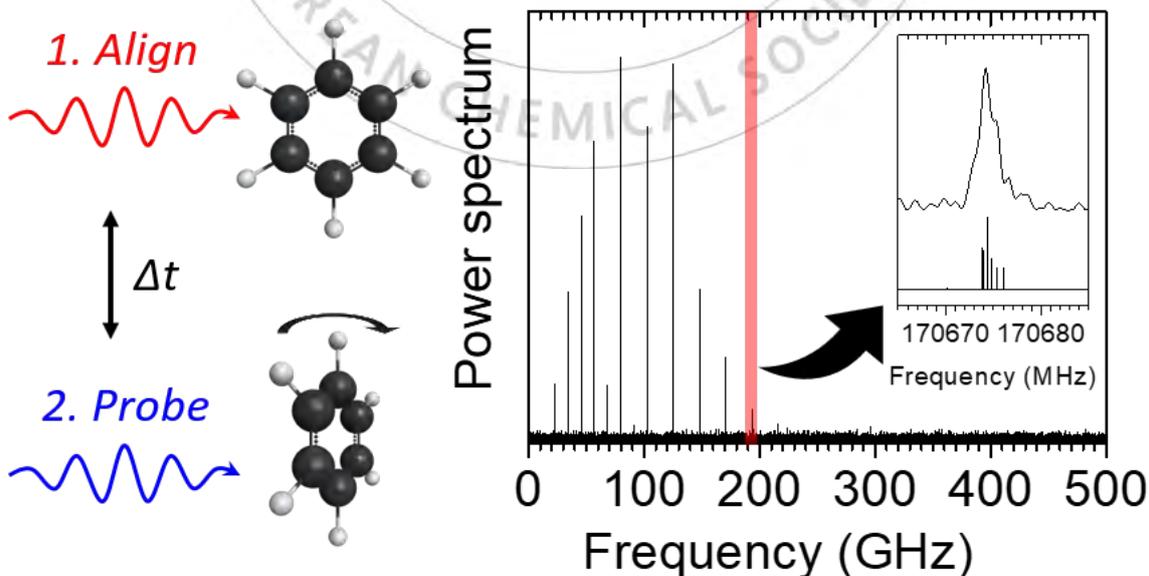
High-resolution rotational Raman spectroscopy of benzene

Jong Chan Lee, Schultz Thomas^{1,*}

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

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

We present a rotational Raman spectrum for benzene with single-MHz resolution, more than a 100-fold improvement on literature data and sufficient to partially resolve K-splitting in some bands. Spectra for a frequency range of 0 to 500 GHz were measured through the observation of a coherent rotational wave packet in the time domain over a time scale of 1 microsecond. Spectroscopic frequencies were referenced to a GPS-stabilized clock. Fitted molecular constants of $B = 5689.2671(\pm 52)$ MHz, $DJ = 1178(\pm 50)$ Hz, and $DJK = -2300(\pm 120)$ Hz agree with results from some high-resolution rovibrational and rovibronic spectra but contradict others.



Poster Presentation : **PHYS.P-228**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

CRASY: The High-Resolution Rotational Raman Spectra of trans-1,3-butadiene and Its Isotopologues in the Vibrational Ground State

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An analysis of the gas-phase rotational spectrum of 1,3-trans-butadiene (BD) and its most abundant isotopologues of outer-¹³C-BD and inner-¹³C-BD was performed by a novel spectroscopic method called mass-correlated rotational alignment spectroscopy (CRASY) [1,2]. The rotational Raman spectra for BD was obtained in a broad spectral bandwidth of 500 GHz. Opto-mechanical delay stage, random sparse sampling and pulse jumping extended the scanned delay range up to 100 ns (equivalent to a 30 ns mechanical delay). We achieved a spectral resolution of 10 MHz, which is a factor of three better than the highest resolution literature Raman spectra (30 MHz). A GPS-stabilized external clock provided an easy method for frequency calibration and we obtained a sub-100KHz accuracy in the rotational constants. We determined the rotational constants of inner-¹³C-BD for the first time. The isotope substitution method of Kraitchman was used for structural calculations of BD. We calculate the C-C bond length and pi-delocalization in BD. References 1. Schröter C, Kosma K, Schultz T (2011) "Crazy: Mass- or electron-correlated rotational alignment spectroscopy", *Science* 333:1011–1015. 2. C. Schröter, J. C. Lee, T. Schultz, "Mass-correlated Rotational Raman Spectra with High Resolution, Broad Bandwidth, and Absolute Frequency Accuracy", *PNAS* 115, 5073 (2018). 3. J. Kraitchman, Determination of Molecular Structure from Microwave Spectroscopic Data, *American Journal of Physics* 21, 17 (1953)

Poster Presentation : **PHYS.P-229**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Super-resolution Stimulated Raman Scattering Microscopy

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Optical diffraction restrict the spatial resolution of Raman scattering microscopy offering a label-free, chemical-specific contrast mechanism based on the intrinsic vibrations of chemical bonds or groups. We aim to develop a new method for super-resolution Raman imaging by implementing the depletion strategy of STED (Stimulated Emission Depletion) microscopy to a stimulated Raman scattering (SRS) technique. In order to reduce the effective focal spot of a SRS signal, we overlap the focal spot with a donut shaped beam that eliminates SRS signal at the periphery of the focal spot. In order to achieve resolution 40%. Our depletion principle is based on the competition of two different stimulated Raman processes on the same molecule. When two SR gains shares the same pump pulse, the two processes become coupled and complete: As one of the Stokes beam intensity increases, the other SR gain is selectively suppressed. We obtained up to 70% efficiency for the depletion of the ring breathing mode of benzene by using the CH stretching mode with 2.1 TW/cm^2 of 1026.5 nm. At the biological damage threshold of 1 TW/cm^2 , the depletion efficiency is 40 % and the expected resolution is 6-fold enhanced from the diffraction limit. We will apply the super-resolution SRS technique to image graphene defects by utilizing the competition between graphene's D and 2D peaks. For this purpose, we mapped the spatial variation of D and 2D bands of graphene monolayer via spontaneous Raman spectroscopy.

Poster Presentation : **PHYS.P-230**

Physical Chemistry

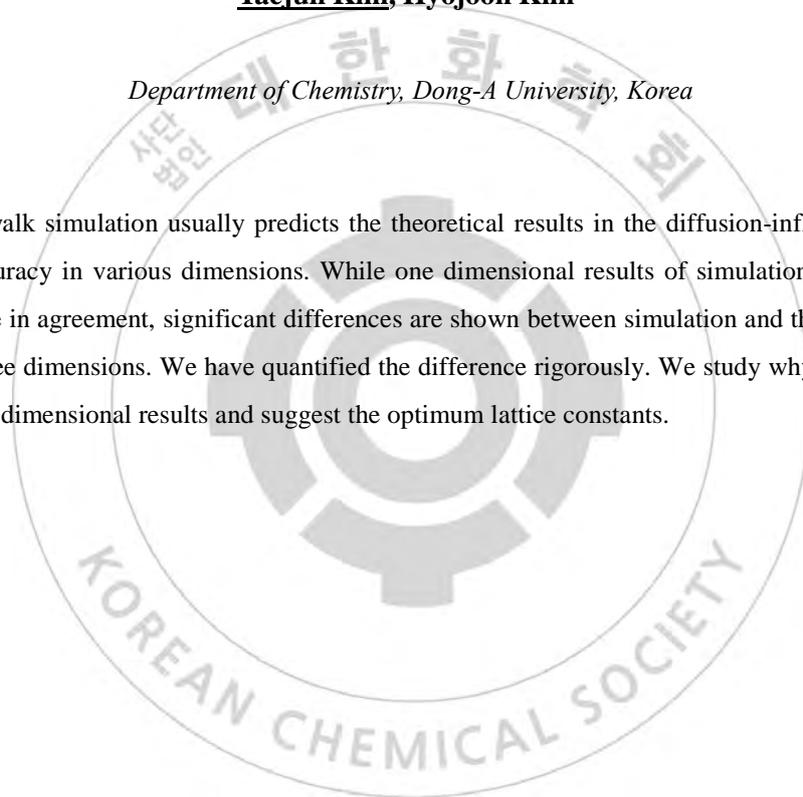
Exhibition Hall 2, FRI 11:00~12:30

Comparison between the Diffusion-Influenced Reaction from the Lattices Constants

Taejun Kim, Hyojoon Kim*

Department of Chemistry, 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-231**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

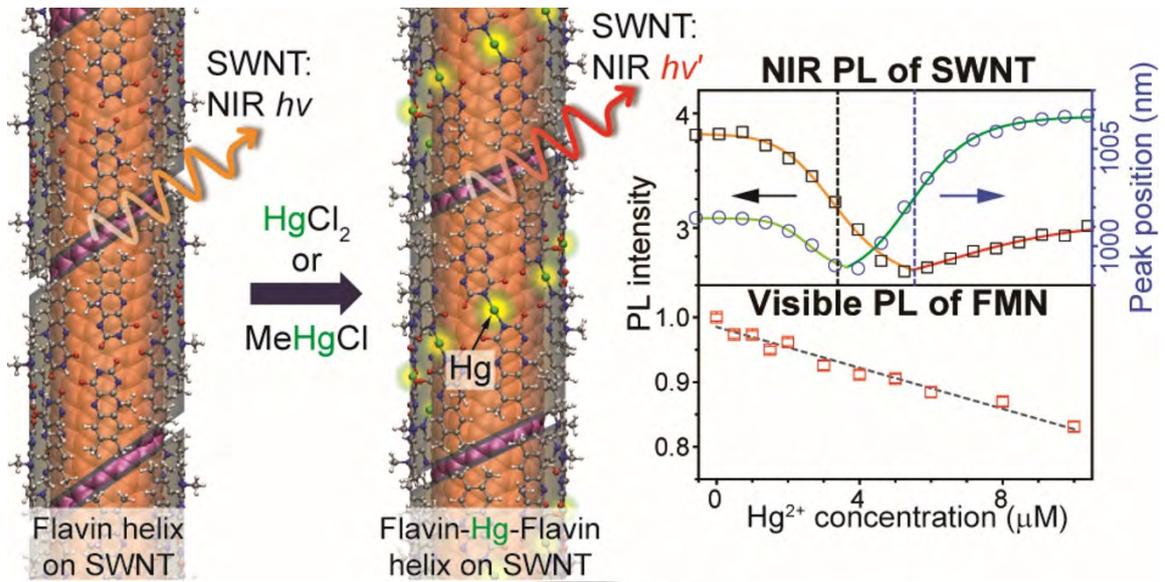
Hg(II)-Selective Probing of Flavin Mononucleotide Helix on Single-walled Carbon Nanotubes via Multimodal NIR Detection

Minsuk Park, Kyeong-Im Hong, Eunji Lee¹, Woo-Dong Jang*, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

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

The development of novel sensing methods for mercury is of paramount importance owing to the impact of this metal on human health and the environment. In this presentation, we observed that flavin mononucleotide (FMN) and its helical motif on single-walled carbon nanotube (SWNT) selectively binds to Hg²⁺ rather than 8 metal ions. Absorption spectroscopy-based stoichiometric studies show that FMN preferentially forms a 2:1 rather than a 1:1 complex with Hg²⁺ at high FMN concentrations. On the basis of the similarity to the thymine-Hg-thymine complex, it is proposed that 2:1 complex between opposing pair of FMN groups and Hg²⁺ comprises a Hg-bridged pair of FMN groups. Upon addition of as little as a few hundred nanomoles of Hg²⁺, binding of FMN-SWNT with HgCl₂ induces changes in absorption and photoluminescence (PL) spectra. Moreover, FMN-SWNT displays simultaneous multiple sigmoidal changes in NIR PL of SWNT having different chiralities with Hg²⁺ addition. Computational calculations indicate that those optical changes originate from Hg-mediated conformational changes occurring on the helical array of FMN on SWNT. HRTEM revealed that the presence of Hg²⁺ in complexes with FMN-SWNT enables visualization of helical periodic undulation of FMN groups without the need for staining. Moreover, circular dichroism (CD) study revealed that FMN-SWNT decreases its dichroic bands upon the addition of Hg²⁺ due to the formation of a centrosymmetric FMN-Hg-FMN triad on SWNT. The use of FMN-SWNT is applied to organomercurials detection to confirm the extensibility. The binding mode specificity and multimodal changes observed in response to Hg²⁺ ions suggest that systems based on FMN-SWNT can serve as *in vivo* NIR beacons for the detection of various mercury derivatives.



Poster Presentation : **PHYS.P-232**

Physical Chemistry

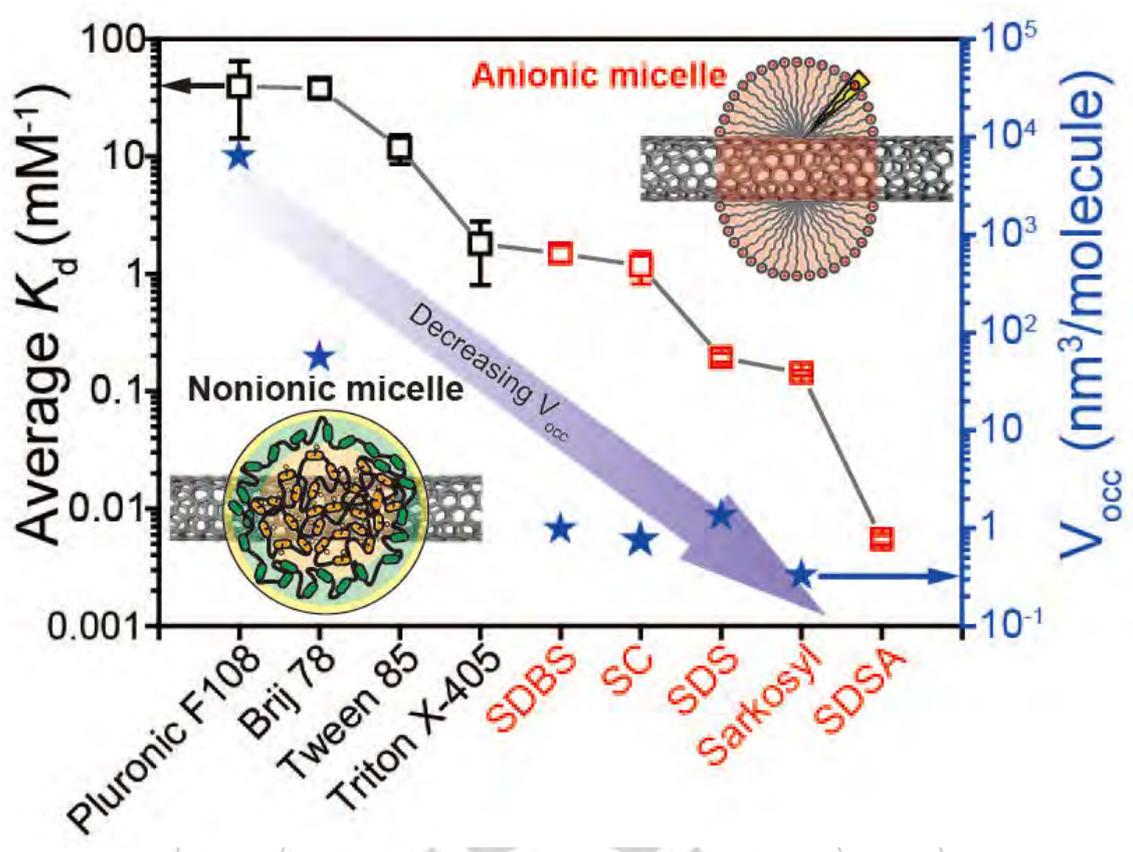
Exhibition Hall 2, FRI 11:00~12:30

Classifying of Binding Affinities and Cooperative Behavior according to Ionic Charge of Various Surfactants on Single-walled Carbon Nanotubes

Minsuk Park, Junmo Park, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Understanding the binding affinity (K_d) of surfactant on single-walled carbon nanotube (SWNT) surface is important in designing the separation method and high-end application. In this presentation, we quantitatively determined the comprehensive K_d and the aggregation number (γ) of nine nonionic/anionic surfactants according to SWNT chirality and some cases of handedness. Sensitive photoluminescence (PL)-based titration using flavin mononucleotide (FMN)-SWNT composites showing the largest redshifted optical transition displayed obvious two-step PL deflection corresponding to partial and full replacements of FMN, respectively. Especially, the second transition exhibited sigmoidal PL trajectories whose midpoint represent the reciprocal of K_d was slightly different from the critical micelle concentration of the surfactant alone, which suggests the enhanced micellization on the SWNT surface. Moreover, nonionic polymeric surfactants displayed larger K_d and lower γ values than those of anionic surfactants due to the differences such as the occupied volume of on the SWNTs, surfactant organization structure, and specificity of the hydrophobic part. Specifically, K_d values between Pluronic F108 and sodium dodecyl sulfonate differed by four orders of magnitude. During the replacement, K_d and γ during the titration were affected by the degree of orderliness of FMN helix on SWNT surface induced by the aging process, leading to a more stable complex. This study suggests that scaling the interactions between surfactant and SWNT by using surfactant replacement provides novel guidelines to design fine-tuned SWNT sorting method that combined by more than two surfactants.



Poster Presentation : **PHYS.P-233**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Flavin-Functionalized Self-Assembled Monolayer Design for Individualized Single-Walled Carbon Nanotube Networks

Junmo Park, Ye Ri Han¹, Minsuk Park, Chul-Ho Jun*, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

¹*Daegu Gyeongbuk Medical Innovation Foundation, Korea*

Single wall carbon nanotubes (SWNTs) are one of the candidates for next-generation semiconducting materials due to their excellent electron mobility and physical robustness. Specifically, controlled immobilization of SWNT networks, which are individualized at specific position, is important in a variety of electronic applications. In this presentation, we report how to synthesize a self-assembled monolayer using Flavin derivatives (Flavin SAM) and immobilize the SWNT network on a substrate non-covalently. The flavin-terminated dimethylsilane is covalently bonded to the silicon dioxide substrate through a direct coupling method or a multi-step method including click reaction. Flavin-SAM adsorbs individualized SWNT dispersions with SDS (sodium dodecyl sulfate), which is widely used as a dispersant, which shows a trend of Langmuir isothermal adsorption. Through atomic force microscopy (AFM), SWNT is confirmed to be partially assembled by the flavin on the substrate, helical wrapping, and monolayer deposition, respectively. It also exhibits strong photoluminescence (PL) of SWNTs present on the substrate despite intimate interactions with the substrate. Moreover, SWNT of flavin-SAM imparts diameter (d_t) selectivity. Finally, to compare the efficient assembly of SWNTs, SWNTs were assembled into patterned SAMs with various functional groups and demonstrated the superiority of Flavin-SAM. This study provides the importance of the molecular design to assemble SWNT network in a customized way.

Poster Presentation : **PHYS.P-234**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The effects of methylated cytosine on the formation of kink on highly bent DNA

Sanghun Yeou, Seong Keun Kim¹, Nam Ki Lee^{1*}

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

¹Division of Chemistry, Seoul National University, Korea

Methylated cytosine (mC) is one of the major factors of gene regulation. For decades, it is well-known that mC influences chromatin accessibility and recruitment of proteins. mC also affects physical properties of DNA like flexibility which is the important parameter of DNA bending for nucleosome in recent study. This means mC may affect directly formation of kink, melted base pairs on middle of DNA structure, which seems to have important role in extreme DNA bending like nucleosome formation. Therefore, we developed D-shaped DNA single molecule FRET based assay for measuring the kink formation of short oligo to observe effects of mC on kink formation. We showed that the more number of mC is, the more the formation of kink enhances. Also, we calculated worm-like chain (WLC) and Freely-joint chain (FJC) model analysis to make sure to the increase of DNA stiffness that can induce kink formation. These results suggested that the bending stiffness increment by mC should lead kink when highly bent.

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Observation of non-canonical bending tendency of DNA oligo using single molecule spectroscopy

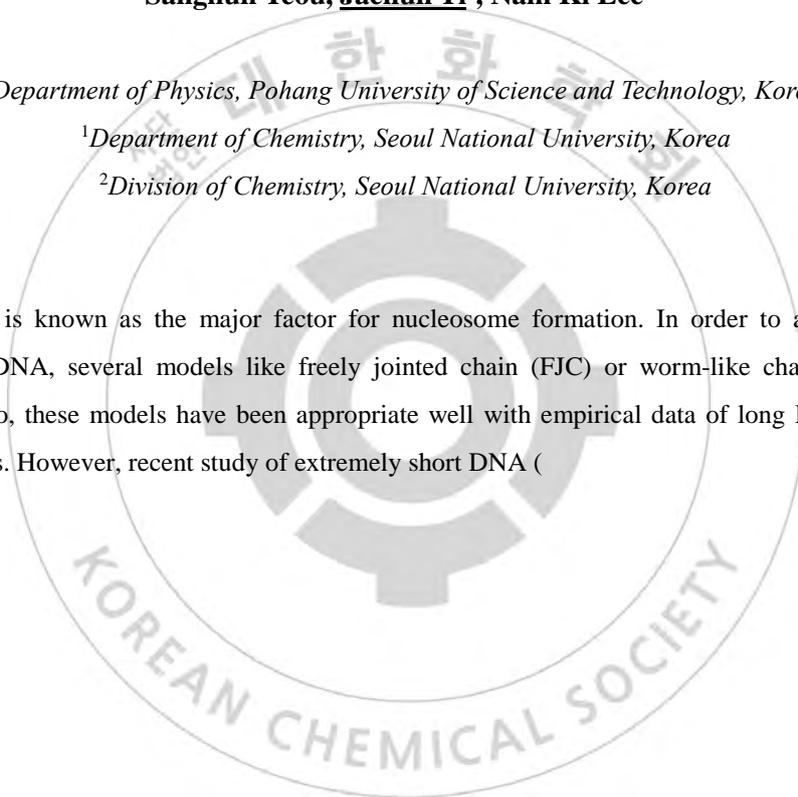
Sanghun Yeou, Jaehun Yi¹, Nam Ki Lee^{2,*}

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

¹Department of Chemistry, Seoul National University, Korea

²Division of Chemistry, Seoul National University, Korea

DNA bending is known as the major factor for nucleosome formation. In order to analyze physical properties of DNA, several models like freely jointed chain (FJC) or worm-like chain (WLC) were suggested. Also, these models have been appropriate well with empirical data of long DNA (~kbp) for several decades. However, recent study of extremely short DNA (



Poster Presentation : **ANAL.P-236**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Shape Effect on the Refractive Index Sensitivity of Localized Surface Plasmon Resonance Inflection Points in Single Gold Nanocubes with Vertices

Ji Won Ha*, **Hui Bin Jeon**

Department of Chemistry, University of Ulsan, Korea

Plasmonic gold nanoparticles with sharp tips and vertices, such as gold bipyramids (AuBPs) and gold nanocubes (AuNCs), have been widely used for high-sensitivity localized surface plasmon resonance (LSPR) sensing. However, conventional LSPR sensors based on frequency shifts have a major disadvantage: the asymmetry and broadening of LSPR peaks because of instrumental, environmental, and chemical noises that limit the precise determination of shift positions. Herein, we demonstrated an alternative method to improve the efficiency of the sensors by focusing on homogeneous LSPR scattering inflection points (IFs) of single gold nanoparticles with a single resonant mode. In addition, we investigated the effect of the shape and vertices of AuNCs on the refractive index (RI) sensitivity of homogeneous LSPR IFs by comparing with gold nanospheres (AuNSs) of similar size. The results show that for both AuNCs and AuNSs, tracking homogeneous LSPR IFs allows for higher RI sensitivity than tracking the frequency shifts of the LSPR peaks. Furthermore, single AuNCs with vertices exhibited higher RI sensitivity than single AuNSs of similar size in the homogeneous LSPR IFs. Therefore, we provided a deeper insight into the RI sensitivity of homogeneous LSPR IFs of AuNCs with vertices for their use in LSPR-based biosensors.

Poster Presentation : **ANAL.P-237**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A study on the determination of inorganic arsenic by solid phase extraction and fs LA-ICP-MS

Seon Hwa Lee, Sang-Ho Nam*

Department of Chemistry, Mokpo National University, Korea

The toxicity of arsenic depends on the concentration and chemical structure present in the natural environment. Thus, the accurate determination of inorganic arsenic in various samples is necessary. IC-ICP-MS (Ion Chromatography-Inductively Coupled Plasma-Mass Spectrometry) is the most popular method for quantitative and qualitative determination of arsenic. However, the method has disadvantages of complex instrument, elaborate sample preparation and long analysis time. In this study, inorganic arsenic species were separated using a membrane filter disk with strong anion exchange in the SPE (Solid Phase Extraction) method, then determined by fs LA-ICP-MS (femtosecond Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry). The detection limit of inorganic arsenic was 0.095 $\mu\text{g}/\text{kg}$ by fs 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 from organic arsenics. The linear dynamic range was from 1 to 1000 $\mu\text{g}/\text{kg}$ by LA-ICP-MS, and the correlation coefficient was 0.99997. The recovery rate of the sample is close to 110%. A new method using solid phase extraction and fs LA-ICP-MS was the accurate and sensitive method for quantitative analysis of inorganic arsenic in a sample.

Poster Presentation : **ANAL.P-238**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Influence of the Capping Material on Chemical Interface Damping Induced by Pyridine with Nitrogen in Single Gold Nanorods

Kyeong Rim Ryu, Ji Won Ha^{1,*}

Chemistry, University of Ulsan, Korea

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

The chemical interface damping (CID) is one of the plasmon decay processes in gold nanoparticles. Herein, to find new functional groups that can induce CID as an alternative to thiol groups, we performed dark-field (DF) scattering studies of gold nanorods (AuNRs) with pyridine as adsorbate. We found that the adsorption of pyridine molecules on single AuNRs through a Nitrogen-Au interaction leads to the increased localized surface plasmon resonance (LSPR) linewidth. However, pyridine molecules were not adsorbed effectively on the AuNR surfaces with the capping reagent on the particle surfaces. Therefore, this study allows us to gain new understanding of the effect and role of the capping reagent in CID induced by pyridine. Furthermore, pyridine with nitrogen, an alternative to thiol groups, was revealed to induce a strong CID in AuNRs through the interaction of nitrogen with the Au surfaces where the capping material was removed by the oxygen plasma treatment.

Poster Presentation : **ANAL.P-239**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development and validation of a sensitive Gas Chromatography-Combustion/isotope Ratio Mass Spectrometric method for anti-doping purposes

Kang Mi Lee

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

The World Anti-Doping Agency (WADA) bans the use of anabolic steroids by athletes for sports performance enhancement. Synthetic copies of anabolic steroids are chemically identical to endogenous steroids, but there are small differences in the ^{13}C to ^{12}C ratios of the synthetic analogues. These differences can be measured using a gas chromatography-combustion isotope ratio mass spectrometry (GC-C/IRMS). However GC-C/IRMS analysis requires an extensive clean-up procedures and a large volume of sample because it can only determine the $^{13}\text{C}/^{12}\text{C}$ ratios of a pure compound. In consideration of limited amount of urine for anti-doping analysis, using large volume of urine can be an issue to meet the requirement sensitivity of IRMS. Therefore, acetylation derivatization is commonly recommended in GC-C/IRMS analysis because acetylated compounds show superior gas chromatographic behavior even acetylation requires much cautions on sample preparation. The aim of this study is to develop and validate a sensitive GC-C-IRMS analysis method using acetylation for anabolic steroids in human urine. The new method was combined with HPLC cleanup and allowed accurate and reproducible results enough to be successfully applied to urine samples that contain low concentration of steroids. Moreover the developed method was fully satisfied with WADA criteria.

Poster Presentation : **ANAL.P-240**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Accurate measurement of total arsenic by considering arsenic species

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

Department of Chemistry, Mokpo National University, Korea

Accurate measurement of total arsenic in a sample has been important as the toxicity related to the arsenic element has been widely known. Total amount of arsenic in a sample has been critical, but the chemical species of arsenic has also been very critical because their toxicity depend on the chemical forms. However, 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. For the quantitation of total arsenic in a sample, arsenic species in a sample have been not considered as far as we know. In general, the standard solution of arsenic has been made by As(V) standard. It might be good for the sample which its major species are As(V). But, if the major species of arsenic in a sample are different from As(V), the arsenic species of the standard solution 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 different arsenic species used in this study were As(V), As(III), MMA, DMA and AsB. The internal standards for the determination of total arsenic in rice and oyster were also investigated in this study. The best internal standard was Tellurium.

Poster Presentation : **ANAL.P-241**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

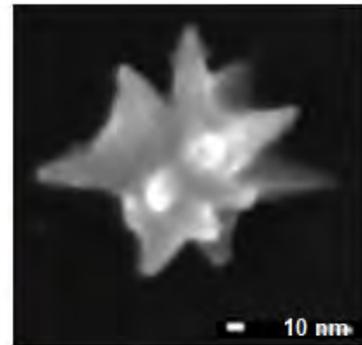
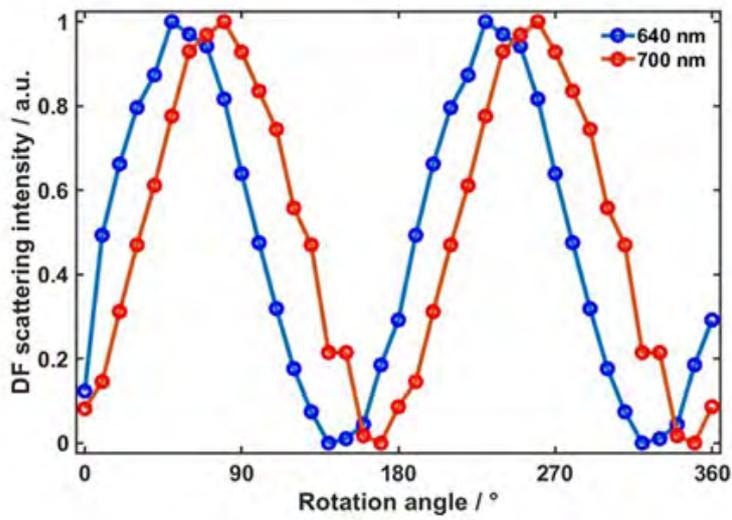
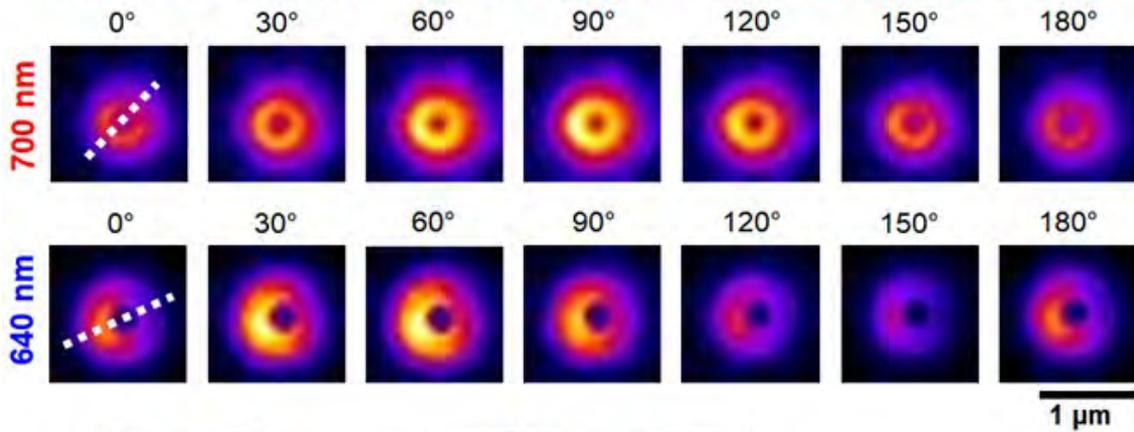
Polarization- and Wavelength-Dependent Defocused Scattering Imaging of Single Gold Nanostars with Multiple Long Branches

Geunwan Kim, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

We demonstrated the polarization- and wavelength-dependent defocused scattering properties of single gold nanostars (AuNSs) with multiple long branches on their surfaces at the localized surface plasmon resonance (LSPR) wavelengths. As a function of the rotational angle of a polarizer, the defocused DF scattering intensities of single AuNS were periodically changed without changing in the doughnut-shaped scattering patterns at two LSPR excitation wavelengths. Furthermore, the characteristic doughnut-shaped defocused scattering pattern enabled to resolve the spatial field distributions of single dipoles on the same AuNS surface at two LSPR wavelengths. Finally, we could track real-time rotational dynamics of a AuNS rotating on a glass slide under defocused microscopy. Therefore, we provided a deeper understanding of the defocused scattering properties of single AuNSs with multiple long branches randomly extended on the surface.

Polarization-dependent Defocused Images of Gold Nanostar



Poster Presentation : **ANAL.P-242**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

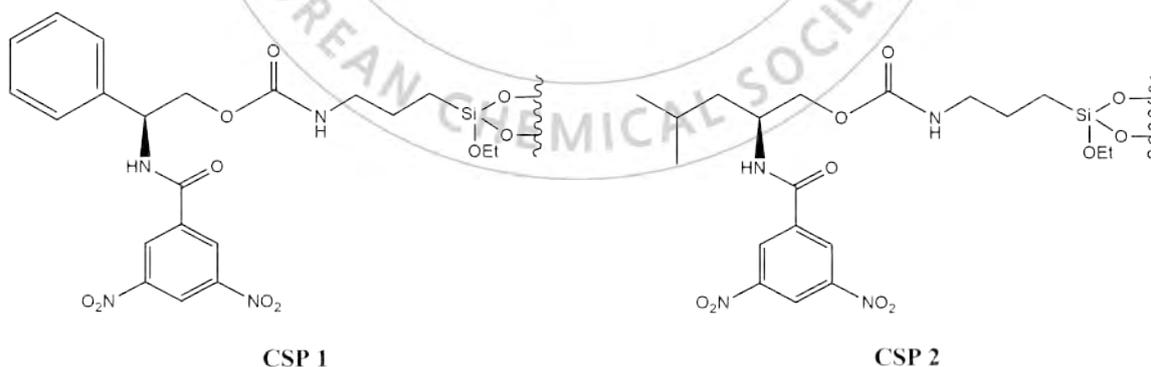
Enantioseparation on 3,5-dinitrobenzoyl amino alcohol derived CSPs by high performance liquid chromatography and supercritical fluid chromatography.

Gyuri Kim, Heo KyuSung, Jae Jeong Ryoo^{1,*}

Department of Chemistry, Kyungpook National University, Korea

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

N-3,5-Dinitrobenzoyl(DNB) phenylglycinol derived CSP(CSP 1) and leucinol derived CSP(CSP 2) were used for the separation of various chiral analytes.^{1,2} In this study, we synthesized the chiral stationary phases using 2 μm silica gel instead of 5 μm silica gel to improve the number of theoretical plate and use for supercritical fluid chromatography, compared the resolution. 1. J. J. Yu; D. H. Ryoo; J. M. Lee; J. J. Ryoo. *Chirality* 2016, 28, 186. 2. J. J. Ryoo; T. H. Kim; S. H. Im; Y. H. Jeong; J. Y. Park; S. H. Choi; K. P. Lee; J. H. Park. *J. Chromatogr. A* 2003, 987, 429.



Poster Presentation : **ANAL.P-243**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Sensitive and Selective Detection of Symmetric Dimethylarginine by Competitive Enzyme-Linked Immunosorbent Assay

Jimin Oh, Insook Rhee *

Department of Chemistry, Seoul Women's University, Korea

Sensitive immunoassay has the unique properties related to complex form of target and binder. It can be fitted to these requirements with simplicity, specificity and sensitivity to accomplish selective assay of target detection. A competitive enzyme-linked immunosorbent assay (ELISA) for detection of symmetric dimethylarginine (SDMA) in serum was developed using the SDMA-HRP conjugate, as a tracer, synthesized via activating the aldehyde groups of horseradish peroxidase (HRP). A various initial molar ratio of HRP:SDMA (1:20, 1:50 and 1:100) was applied. And then, we evaluate the sensitivity and selectivity of this assay. Firstly, to assess the sensitivity, we chose 1:100 ratio conjugate and observed the best sensitivity with the LOD: 1.15×10^{-10} M. Secondly, to appraise the selectivity, we used various cross-reactants having similar molecular structure to SDMA such as asymmetric dimethylarginine (ADMA), methyl arginine and L-arginine. This new method shows high selectivity for SDMA and none of the cross-reactants show the cross-reactivity. SDMA, the structural isomer of ADMA, is a methylated derivative of the amino acid L-Arginine and is strictly eliminated by renal extraction. In the past, creatinine was the most common bio-marker of renal function, especially glomerular filtration rate (GFR). However, SDMA has been shown more sensitive than creatinine because of the imperviousness to the physical factors and the earlier increasing with chronic kidney disease (CKD). Thus, we expect that this developed method can be a novel approaches for the determination of SDMA and early diagnosis of CKD.

Poster Presentation : **ANAL.P-244**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

N-Doped Carbon Dots for Dual Mode Detection with Large Dynamic Range in analysis of Ag⁺ Ion

Kim Shinik, Weekyung Kang*

Department of Chemistry, Soongsil University, Korea

Recently, carbon quantum dots have attracted attention as various advantages such as chemical inertness, lack of blinking, variable fluorescence emission, low cytotoxicity and good biocompatibility as compared with semiconductor quantum dots and organic dyes. In addition, CQD doped with heteroatoms have local surface chemical and electronic properties, thus having adjustable properties in biosensors and bioimaging. We synthesize N-doped carbon quantum dots by urea and citric acid in a single-stage microwave synthesis. The N-doped carbon quantum dots were characterized by TEM, FTIR, fluorescence spectrophotometer and uv - visible spectrophotometer. The N-CQDs exhibit fluorescence characteristics in excitation wavelength-dependent emission and strong fluorescence excitation bands are present at 360 nm and 440 nm.

Poster Presentation : **ANAL.P-245**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of aging on lipidomic changes in mouse serum, kidney, and heart

Jung Yong Eum, JongCheol Lee¹, Myeong Hee Moon^{1,*}

Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Aging is defined as the gradual decline of metabolic functions and is becoming the global burden due to the extended human life expectancy. The detailed metabolism of aging is still not fully understood, but it is well known that aging causes intracellular accumulation of reactive oxygen species which could develop age-related diseases such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Since changes in lipid metabolism may induce these diseases, examining the alteration of lipid levels is important. In this study, using serum, kidney, and heart from the 4- and 25-month-old C57BL6 female mice, a comprehensive lipidomic analysis was done to elucidate age-induced perturbation of lipid profiles by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Among 542 identified lipid species, 279 lipid species were quantified in selected reaction monitoring mode. While most of the lipid species with significant changes (> 2 -fold, $p < 0.01$) were found to be decreased by aging, triacylglycerols were increased in mitochondria rich tissues, especially in the heart. The ratio of phosphatidylcholine over phosphatidylethanolamine (PC/PE) which was the important factor of mitochondria membrane integrity was found to be significantly decreased only in kidney. This presentation demonstrates that nUHPLC-ESI-MS/MS analysis can determine the lipid species showing significant changes in serum, kidney, and heart of aged mice.

Poster Presentation : **ANAL.P-246**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Comprehensive analysis of polyglycerophospholipids by isotope-labeled methylation method

JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Polyglycerophospholipids (PGPLs) refer to phospholipids (PLs) having two or three glycerol moieties and are generally synthesized from phosphatidylglycerol (PG) as a precursor. PG, bis(monoacylglycero)phosphate (BMP), hemi BDP, and bis(diacylglycero)phosphate (BDP) with two glycerols, and dilyso-cardiolipin (DLCL), monolysocardiolipin (MLCL), and cardiolipin (CL) with three glycerols belong to PGPLs. Since these lipids are closely related to each other and regarded as biomarkers with high selectivity in various diseases rather than other PLs, simultaneous analysis of PGPLs is required to understand their pathological roles. In this study, methylation of PGPL was introduced to increase the improvement of separation and MS detection of PGPLs and their regioisomers, and then the isotope labeled methylation (ILM) method was applied for the relative quantitations of PGPLs using nUHPLC-ESI-MS/MS. The efficiency of methylation for PGPLs was higher than > 97% for all of species and ILM method enhanced the S/N ratio of most PGPLs including newly identified species (regioisomers of hemi BDP, DLCL, and MLCL), which were not detected before methylation. The molecular structures of regioisomers can be distinguished by their retention time differences and characteristic fragment ion spectra. When SH-SY5Y cells with and without the drug treatments to induce Parkinson's disease model were analyzed by ILM method, a total of 230 PGPLs including 16 hemi BDP, 71 MLCL and 121 CL species were identified, which is the record breaking number of analyzed PGPLs so far. Furthermore, seven CL species having arachidonic or docosahexanoic fatty acid chains were found to be up-regulated upon drugs treatment, which is an indicative of CL remodeling process in Parkinson's disease model.

Poster Presentation : **ANAL.P-247**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Separation of plasma exosomes and lipoproteins 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

Recently, exosomes are of a great interests due to the possible roles in developing biomarkers for disease diagnosis and prognosis. Exosomes are extracellular vesicles (30 – 150 nm) that are found in blood, urine, and biological fluids, and play important roles in cell signaling. Lipoproteins in blood which carry lipids throughout the body are classified as high-density lipoprotein (HDL, 5 – 15 nm), low-density lipoprotein (LDL, 18 – 28 nm), and very low density lipoproteins (VLDL, 30 – 80 nm). However, it is challenging to isolate exosomes from blood sample due to the presence of lipoproteins. . Field-flow fractionation (FFF) is an analytical technique that separate particles from nano to micron size in an open channel space without packing materials, which is advantageous for separating biomolecules. This study attempts to separate exosomes and lipoproteins in blood plasma samples by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) using field programming with a UV detection (UV) and multi-angle light scattering (MALS) detections. Exosomes and lipoproteins that were fractionated by FI-AF4 were identified by Western blot and transmission electron microscope (TEM).

Poster Presentation : **ANAL.P-248**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optimization of nanoflow ultrahigh performance liquid chromatography (nUHPLC) conditions for high-throughput and rapid lipid analysis by ESI-MS/MS

Gwang Bin Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Since separation in the nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS) is carried out at nanoflow rate regimes, performances of separation can be improved with the increased resolution with the minimization of sample amounts to be injected and the consumption of organic solvents. However, when a large number of sample analysis is required, a high speed separation is necessary for nUHPLC compared to the typical gradient elution condition that requires 30 min for a separation of lipids with broad classes without incurring spectral congestion in MS detection. This study demonstrated that high-throughput and rapid lipid analysis can be carried out within 10 minutes of separation by adjusting gradient elution condition with the increase of flowrates but without increasing the spectral congestion. The average peak width can be decreased to 0.14 min for PC 16:0/16:0 in a 10 min run condition compared to 0.15 min for a 30 min run condition with the standard deviation of retention time in repeated measurements as 1.68 s. The plate numbers of PC 16:0/16:0 can be above 330,000. In addition, MS detection efficiencies of lipid species upon increasing separation speed was evaluated with lipid standards spiked to a serum sample.

Poster Presentation : **ANAL.P-249**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Investigation of changes in serum lipid levels upon the partial hepatectomy of swine in relation to the post-hepatectomy liver failure using nanoflow UHPLC-ESI-MS/MS

HaeA Kim, JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Post-hepatectomy liver failure (PHLF) is the inability of the liver to perform its normal synthetic and metabolic function after liver resection to treat diseases like hepatocarcinoma. Despite much progress in hepatectomy, PHLF still has high morbidity and mortality. Therefore, PHLF is still a serious complication and a possible diagnostic method in its early development stage after surgery is required to be developed. In this experiment, the changes in serum lipid levels of swine serum were investigated according to the degree of liver resection and elapsed periods after operation using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS). Serum samples were collected at four time intervals: before the operation, after 14 hours, 30 hours, and 48 hours of partial hepatectomy operation from six sham swine which did an only laparotomy, seven swines with 70% partial hepatectomy (70% PHx), and seven PHLF swines (90% PHx) which underwent 90% partial hepatectomy. A total of 151 phospholipids, 22 sphingolipids, and 204 glycerolipids were structurally identified based on collision-induced dissociation (CID) experiments and each lipids species of individual serum sample was quantitatively analyzed using selective reaction monitoring (SRM) mode. The alterations in lipid levels between 70% PHx group and 90% PHx groups were statistically evaluated to discover candidate marker species showing significant differences.

Poster Presentation : **ANAL.P-250**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Profiling of lipoproteins from post-menopausal patients with osteoporosis by asymmetrical flow field-flow fractionation and nUHPLC-ESI-MS/MS

Kang Geun Lee, Joon Seon Yang¹, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

¹*The Resource Center for Stable Isotope-Resolved Metabolomics, University of Kentucky, United States*

Pathological mechanism of osteoporosis is not clearly known, but osteocytes affected by oxidized lipids are expected to be one of major factors. Bone mineral density (BMD) reaches the highest level in the age of 30s and decreases slowly over time, but symptoms are scarcely detected and it already gets serious when found out. Lipids play important roles in signal transduction, cell formation and various cellular processes. therefore, they are expected to be possible biomarkers to several diseases. Therefore, it is important to study relationships between lipids consisting lipoproteins in plasma and osteoporosis for early diagnosis. There are several studies about the relationship between lipids and osteoporosis in which BMD showed a meaningful correlation with low-density lipoprotein (LDL) and high-density lipoprotein (HDL). However, none of them conducted quantitative and qualitative analysis by using mass spectroscopy to differentiate lipid species at the molecular level in detail. In this study, 39 female plasma samples were classified into three groups : women having osteoporosis with no history of other diseases (n=10), women having osteoporosis with history (n=7), and age-matched control (n=22). Flow field-flow fractionation (FIFFF) is a technique that can separate particles or macromolecules by size. Lipoproteins of blood samples were fractionated by sizes using asymmetrical flow field-flow fractionation and the lipids were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Overall, 341 lipids from patient's plasma were identified and 289 lipids were quantified with statistical evaluations for the screening species with significant alterations when osteoporosis was developed.

Poster Presentation : **ANAL.P-251**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Charge effect of ATP on changing self-assembly mechanism of amyloidogenic proteins

Chae Eun Heo, Jong Yoon Han, Sooyeon Chae, Chae Ri Park, MyungKook Son, Min Ji Kim, Dongjoon Im, Paul Valery Migisha Ntwali, Gyeongseo Min, Chaehyeon Yoon, Hugh I. Kim*

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Amyloid fibrillation is a biological process by which amyloid disease-related protein molecules are self-assembled by hydrophobic interactions. In human body, such amyloidogenic proteins (e.g. amyloid- β , α -synuclein, human islet amylin polypeptide, tau, lysozyme and insulin) exist with specific charge state, positive or negative, depending on their inherent isoelectric point. To build a well-aligned fibril by assembling same charged proteins, it must overcome the electrostatic repulsion between the same charged residues. Thus, numerous research has been reported that charged species abundant in our body (e.g. metal ion, DNA, nucleic acid, heparin, glycosaminoglycans etc.) influence to the mechanism of amyloid fibrillation by electrostatic interaction. Here, we have studied to understand the molecular mechanism of protein fibrillation under ATP, which is a small biological polyanion and is present in high levels in cell. Firstly, we have conducted the thioflavin T(ThT) assay which monitors the formation of amyloid fibril. To identify and characterize the protein complexes between protein and small molecules, we have utilized electrospray ionization mass spectrometry (ESI-MS) and ion mobility spectrometry (IMS), along with circular dichroism (CD) and solution small-angle x-ray scattering (SAXS). The experimental evidence obtained from these diverse analytical techniques, and subsequent studies about biological anion-mediated protein aggregation would be highly helpful in understanding the mechanistic details of amyloid fibrillation under the influence of external factors, which affect protein-protein interactions.

Poster Presentation : **ANAL.P-252**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Cure Monitoring and Adhesion Characterization of Epoxy Powder Coatings using Time-Domain NMR Relaxometry

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Epoxy powder coatings are eco-friendly coatings composed of 100% solids without any solvents, and widely used in the industrial field because of their excellent corrosion resistance and flexibility. In particular, the epoxy powder coatings for steel pipes improve the durability by protecting pipes from various corrosive environments such as moisture, dissolved oxygen, and bacteria. The failures such as water absorption or delamination of epoxy coatings are associated with the curing reaction and adhesion properties. Therefore, it is important to monitor the curing reaction to investigate the reaction rate and flow properties of the steel surface. We selected various epoxy resin types and observed the curing behavior using DSC. Also, time-domain NMR (TD-NMR) was used to confirm the flow characteristics through solid and liquid phase ratio during cure reaction. The adhesion test of coated specimens with hot water was conducted and compared with results from TD-NMR. We observed that the longer the spin-spin relaxation time, the better the fluidity on the steel surface during curing and the better the adhesion of the final cured coating.

Poster Presentation : **ANAL.P-253**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Analysis of flame retardant content in fire proof coating

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Fire proof coating is painted on steel frames and wood to prevent the building from collapsing or spreading in the event of a fire. When a fire occurs in a building painted with fire proof coating, a char is formed, and an inert gas expands the film of paint to form a foam layer. The flame retardant content in fire proof coating is about 30~40%, and melamine, ammonium polyphosphate and pentaerythritol are mainly used. The mixture ratio and content of flame retardant components result in different foaming efficiency and refractory performance of the paint. Standardization of flame retardant quantitative analysis method is required to optimize design mix of fire proof coating. In this study, we established optimal extraction conditions of flame retardant in fire proof coating through recovery rate evaluation using liquid- liquid extraction method. Quantitative analysis of flame retardant was performed using LC-MS MRM mode.

Poster Presentation : **ANAL.P-254**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Comparison of phase content analysis methods of gypsum

Jiyeon Lee

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Gypsum board is a natural material that is used as a building material with the characteristics of insulation and light weight, environment friendly. It is consist of calcium sulphate dihydrate ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), calcium sulphate hemihydrates ($\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$) and calcium sulphate anhydrite (CaSO_4). Depending on the content of $\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$, it may affect the properties of the gypsum board products. To analyze phase contents, there are methods using thermal changed by reaction, losing weight by heat, and diffracted x-ray from sample. To figure out the best method having short time, accurate results, and simple process, we have compared all factors and results of those methods. In this study, we experimented all methods and found the reason why the phase and content differences were occurred, and the analysis limitations of each methods. Finally, the result using rietveld method is the closest to standard value. And the limit of phase analysis is less than other methods. It is powerful function to analysis of impurities in gypsum materials. Through this result, rietveld method is expected to widely apply to inspection of gypsum materials.

Poster Presentation : **ANAL.P-255**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

One-pot Synthesis of Silicon Nanoparticles for Hyperpolarized ^{29}Si Magnetic Resonance Imaging

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Silicon nanoparticles (Si NPs) has developed for application in medicine because of their biocompatibility, biodegradability, drug loading and imaging agents. Herein, we report a solution synthesis of Si NPs as hyperpolarized magnetic resonance imaging. The Si NPs was synthesized by the reduction of silicon tetrachloride using organic reductants at low temperature. This nanoparticles size and dispersity were controlled by investigation ratio of silicon precursor to reductant, temperature and various reducing agents. The chloride-terminated Si NPs was converted to hydroxy-terminated through methoxy-capped. And finally, hydroxyl group was altered by (3-aminopropyl)triethoxysilane (APTES) for enhancing the hydrophilicity and biocompatibility. The morphology, structure and physical properties of Si NPs were confirmed by transmission electron microscopy (TEM), X-ray diffraction (XRD), infrared spectroscopy (IR spectroscopy) and dynamic light scattering (DLS). This research recommends that controlling the size of silicon nanoparticles via colloidal synthesis as the contrast agents for hyperpolarized ^{29}Si magnetic resonance imaging.

Poster Presentation : **ANAL.P-256**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Biodegradable Microcapsule Studies Available in Industry and Bio-application

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Microcapsules have been attracting attention as a means of releasing a functional substance to a target area or protecting it from an external environment by imparting a functional substance capable of exhibiting a desired function in various ways. Although microcapsule research has been conducted in a wide variety of fields, recently, environmental pollution caused by microplastics commonly used in the synthesis of fabric softener has become a serious problem. Therefore, we have attempted to develop a biodegradable microcapsule that solves the environmental problems and is expected to be effective in bioapplication such as drug delivery. In order to make the microcapsules biodegradable, we measured the biodegradability of various microcapsule precursors such as starch and vinyl alcohol by BOD / COD ratio. The microcapsules were synthesized by O/W based interfacial polymerization and it was confirmed that the size could be controlled by stirring speed. The isocyanate is a substance that can give a strong stimulus to the human body, so the residual isocyanate was measured by FT-IR and NMR. In later studies, further evaluation and bench scale experiments will be conducted to enable direct application as a fabric softener, and drug delivery studies will be conducted using bioapplication based on the biodegradable microcapsules synthesized. **Keywords:** Biodegradable microcapsule, interfacial polymerization, textile softener

Poster Presentation : **ANAL.P-257**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Single Bubble Microextraction Coupled with Capillary Electrophoresis

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Headspace (HS) extraction is a technique that have been developed for analysis volatile compounds. In conventional HS extraction, analytes evaporated from a donor phase (acidic) to the headspace and can be enriched to an acceptor phase (basic). The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus a small acceptor volume is preferred. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME) coupled with CE using a basic run buffer solution inside capillary as an acceptor phase. To reduce the headspace area, and increase enrichment factor enriched in more smaller headspace, here we present a new technique, single bubble microextraction (SBME) coupled with CE. It is a simple technique and easy to conduct HS extraction of a small volume sample for CE analysis. To reduce the headspace area, a small air bubble was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor vial. Then, SBME-CE was performed using the acceptor plug remained in the capillary. All steps of SBME-CE were carried out automatically using a commercial CE instrument without any modification.

Poster Presentation : **ANAL.P-258**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile method to fabricate viscoelastic nanocomposites based on supramolecular gels and boron nitride nanotubes via one-pot melt-blending

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We herein report a facile, cost-competitive, and scalable method for producing viscoelastic nanocomposites using supramolecular gels and boron nitride nanotubes (BNNTs) in polymer matrix. by simple mixing. Unlike carbon nanotubes (CNTs), BNNTs has been proposed as a nanocarrier and nanotransducer in the biomedical field because enhanced chemical inertia prefers biocompatibility. In addition, BNNTs demonstrates the potential for aerospace applications due to their shielding properties of strength and radiation. When mixed, a non-volatile eutectic liquid (EL) produced by brief blending of two chemical reagents with simple chemical structures. enabled not only the gelation of BNNTs (EL-BNNTs) but also the dissolution of a number of commodity polymers. To make use of these advantages, viscoelastic nanocomposites were produced via one-pot melt-blending the EL and BNNTs with polyurethane(PUR) and epoxy and their properties have been investigated

Poster Presentation : **ANAL.P-259**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

HPLC-UV Determiation 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 (DES-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, volume of acetic anhydride, time of derivatization, type of basic solution for derivatization, and the effect of salt. Chromatographic separation with HPLC/UV-vis was performed using the Innoval ODS-2 (4.6 mm id × 150 mm length, 5 μm particle size) column and gradient elution mode using water and methanol.

Poster Presentation : **ANAL.P-260**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Microextractoin chromatography for determination of a mixture of ^{90}Sr and ^{90}Zr

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We introduce a method to determine ^{90}Sr and ^{90}Zr using microextraction chromatography system with a column containing Eichrom Sr ResinTM. Due to the stable isobaric interference of ^{90}Zr by ICP-MS, the measurement of ^{90}Sr was difficult. We propose that the method is to separate prior to ICP-MS using microextraction chromatography besides the low volumes inherent to ICP-MS allow for decreasing radioactive wastes production. In our system, the volume of sample injection into the extraction column is 270 μl . Zirconium is passed through the column using 3 M HNO_3 while strontium is retained on the column. Then the strontium is eluted with 1% acetic acid. Total flow rate is about 100 $\mu\text{l}/\text{min}$. After extraction, the quantitation is achieved by ICP-MS. The recoveries are $91.0\% \pm 0.7\%$ and $96.1\% \pm 0.9\%$ for strontium and zirconium, respectively.

Poster Presentation : **ANAL.P-261**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development and validation of anabolic steroids screening method for anti-doping with gas chromatography/tandem mass spectrometry

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Anabolic androgenic steroids (AAS) are the major class of doping agents and their consumption produces adverse effects involving several organs and system diseases. The World Anti-Doping Agency (WADA) encourages drug testing laboratories to develop anabolic steroids screening methods which can determine a large number of compounds at very low detection levels in urine. In this study, new screening method for the urinary detection of anabolic steroids has been developed and validated using gas chromatography/tandem mass spectrometry (GC/MS/MS). The method takes advantage of enhancing selectivity, sensitivity and efficiency compare to using gas chromatography mass spectrometry (GC/MS). More than 100 substances including endogenous and exogenous steroids could finally be monitored in 16 min with low concentrations in accordance with the minimum required performance levels of the World Anti-Doping Agency. The selectivity of the method showed that no interfering peaks were observed at the retention time of the analytes. Moreover, most of the compounds showed highly satisfactory intermediate precision (< 25%). The optimized method was successfully applied to doping analysis of PyeongChang winter olympic games.

Poster Presentation : **ANAL.P-262**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Preparation of lithium iron pyrophosphate as cathode material for lithium ion battery

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Lithium-ion batteries are the most important energy storage system for wide applications in electronic portable devices and electric vehicles. Among cathode materials, the olivine structured lithium iron phosphate (LiFePO_4), has low cost, low toxicity, high thermal stability and high relatively high theoretical specific capacity. However, its poor high-rate performance of this material restricts its use in large-scale application owing to its low electronic conductivity and slow lithium-ion diffusion. As an alternative cathode material, $\text{Li}_2\text{FeP}_2\text{O}_7$ consisted by pyrophosphate (P_2O_7)⁴⁻ is driven by their thermal stability and improved safety. Pyrophosphate has a two-dimensional lithium diffusion channel and capability to extract more than one lithium ion per formula unit. Iron-based pyrophosphate has cyclic voltammetry (CV) peaks that appear $\text{Fe}^{2+}/\text{Fe}^{3+}$ redox couple at the range of 3.5 ~ 4.0V. In this study, anion doping like fluorine anion is adopted to improve the electrochemical property through the improvement of conductivity. The electrochemical properties of samples were investigated through lithium extraction/inserting processes using galvanostatic charge/discharge and CV measurements to investigate for Li^+ transferring between the electrode materials. Also, solid-state ^7Li NMR have been observed to characterize the structural transformation.

Poster Presentation : **ANAL.P-263**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhanced electrochemical performance of LiFeBO₃ cathode material via anion doped for lithium ion battery

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Anion-doped LiFeBO₃ cathode material has been successfully synthesized by solid-state method followed heat treatment. Fluorine was used as doping element to improve the conductivity of LiFeBO₃ material. Various amount of fluorine are given during preparation to reach optimum electrochemical performance. The structure of anion doped LiFeBO₃ are investigated by X-ray diffraction, ⁷Li magic angle spinning NMR spectroscopy, and Fourier Transform Infrared spectroscopy. Also, the electrochemical test and cyclic voltammetry are performed by galvanostatic charge and discharge test. The result showed that fluorine-doped LiFeBO₃ has effectively improved electrochemical performance.

Poster Presentation : **ANAL.P-264**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

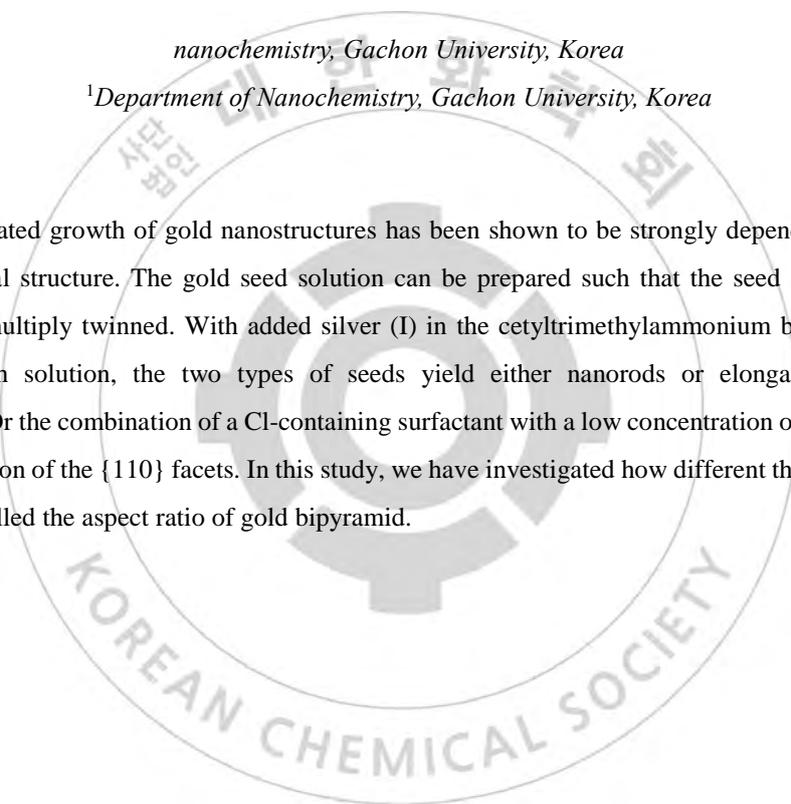
Various Multi-Facet Gold Bipyr amid Fabrication

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The seed-mediated growth of gold nanostructures has been shown to be strongly dependent on the gold seed nanocrystal structure. The gold seed solution can be prepared such that the seed are either single crystalline or multiply twinned. With added silver (I) in the cetyltrimethylammonium bromide (CTAB) aqueous growth solution, the two types of seeds yield either nanorods or elongated bipyr amidal nanoparticles. Or the combination of a Cl-containing surfactant with a low concentration of Ag plays a role in the stabilization of the {110} facets. In this study, we have investigated how different these solutions are and how controlled the aspect ratio of gold bipyr amid.



Poster Presentation : **ANAL.P-265**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Electrochemical study of fluorine doped lithium vanadium borate as a cathode material for lithium ion battery

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Recently, lithium transition metal borates, LiMBO_3 ($M = \text{Mn, Fe or Co}$), have been studied by many research groups due to low weight of $(\text{BO}_3)^{3-}$, relatively weak B-O bond, and high theoretical capacity. Its weaker B-O bond makes fast lithium ion diffusion. However, it has limitation because of their low ionic and electronic conductivities, which is revealed relatively low reversible capacity. Therefore, LiV_2BO_5 (LVBO) has been studied to improve operating potential, because multiple valence states of vanadium element can provide a high theoretical energy density. Also, fluorine doping in LVBO has been attempted to synthesis by sol-gel method. The morphology and composition of materials have been identified with scanning electron microscope and X-ray diffraction. The electrochemical properties are characterized by using galvanostatic charge/discharge and cyclic voltammetry measurements. The optimum doping ratio in LVBO is still under study with electrochemical properties.

Poster Presentation : **ANAL.P-266**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Infrared spectroscopic characterization of bile juices acquired from patients with gallbladder diseases

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Bile juice is a body fluid related with emulsifying and micellizing cholesterol in intestine, secreted in liver and stored in gallbladder (GB). Composition of bile juice would be different by health conditions of each patient; therefore, bile juice could be a beneficial medium for studying GB diseases. In this study, infrared (IR) spectroscopy has been used to study bile juices from patients of GB polyp and GB cancer. Before IR measurement, raw bile juice samples were pretreated with chloroform-methanol mixture solution to extract and separate organic, aqueous and protein agglomerates. Then, each phase-separated sample was dropped on hydrophobic OTS (octadecyltetrachlorosilane)-coated Si wafer to form reproducible circular droplet and dried for IR spectral acquisition. IR spectra were collected across a dried sample (line-mapping) and a representative spectrum was selected among the mapped spectra for further examination. In the chosen spectra, key spectral features related with GB polyp and GB cancer were searched and characterized. Next, to examine potential of IR spectroscopic discrimination of bile extracts according to diseases, principal component analysis (PCA) was used to reduce dimensions of spectral data into simply 2- or 3-dimensional score domains to easily recognize potential differences between GB polyp and cancer samples. In final, the future direction of this research will be discussed.

Poster Presentation : **ANAL.P-267**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spatially offset based Raman scattering-based line-mapping as means to determine sample particle size

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Spatially offset based Raman scattering (SORS)-based line-mapping has been evaluated as a means for determining sample particle size. In SORS measurement, the position of Raman photon collection is away from that of laser excitation. As previously studied, the distribution of Raman photons became broader with the increase in particle size, as the mean free path of laser photons, the average photon travel distance between consecutive scattering locations, became longer under this situation. Therefore, when a SORS line mapping is performed along a packed powder sample, the peak intensities of sample in a series of the mapped spectra expect to decrease as offset distance becomes longer. Moreover, the slope in the change of intensity would be related with particle size, such as a greater slope for larger particle size. This possibility was the driving force for this research. For investigation, polyethylene (PE) powders with different particle sizes (300-200, 200-150, 150-100 and 100-75 micron) were prepared and SORS-line mapping was performed for each sample. Then, the slope of peak intensity was examined in relation with sample particle size. Various samples with different densities and refractive indices are under evaluation for deeper exploration.

Poster Presentation : **ANAL.P-268**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Feasibility of electrochemically modulated SERS measurement for improved differentiation of gallbladder diseases

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A screen-printed electrode (SPE) covered with three-dimensional gold nanodendrites (AuNDs) was used to measure SERS spectra of bile juices. To acquire SERS spectra with distinct features, a bile juice was pretreated with CH₂Cl₂-CH₃OH solution to eliminate hydrophobic components such as lipids and the remained aqueous hydrophilic phase was measured. Interestingly, Raman spectral features of the aqueous phase samples mostly resembled with those of bilirubin. So, it was presumed that the peaks were originated from conjugated-bilirubins, formed in a liver by attachment of sugars (such as glucuronic acid) to bilirubin (a heme break down product). Subsequently, conjugated-bilirubin becomes soluble in water. It expects that structure and composition of conjugated-bilirubin are dissimilar depends on different GB diseases (GB stone, polyp and cancer). Further, potentially improve the differentiation, varying electrochemical potentials were applied to the bile juice sample on SPE surface and corresponding SERS spectra were also acquired. Finally, principal component analysis (PCA) was used to qualitatively evaluate the degree of discrimination among these 3 GB diseases in the cases with and without application of electrochemical potential.

Poster Presentation : **ANAL.P-269**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Superlocalization of Single Tumor Necrosis Factor- α Molecules on Nano-Region Using 3D Enhanced Dark-Field Nanoscopy

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Superlocalization on nano-region by the least-cubic algorithm of biomarker was performed using three dimensional (3D) enhanced dark-field nanoscopy. The tumor necrosis factor- α (TNF- α) with nanotag (silver) as a biomarker was immunoreacted on 100 nm gold nanospot. The localization precision and sensitivity with a least-cubic algorithm provided accurate position information for the immunotargeted site on 100 nm gold spot. The accurate localization of the nanoparticle for detection (i.e., silver and gold) after reaction provided important information to reduce the error in data interpretation as well as the presence or absence of reaction. Especially, negligible signals were observed using interfering proteins without cross-reactivity, showing the high specificity of the system for single biomolecule detection.

Poster Presentation : **ANAL.P-270**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Single-Molecule Nanocatalysis for Location Effect of Gold Nanoparticle on Carbon Nanotube

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Gold nanoparticles were immobilized on carbon nanotubes by two ways: filling of Au nanoparticles inside the CNT channels (Au/CNTs-in) by capillary action and dispersion of Au nanoparticles on the exterior surfaces of CNTs (Au/CNTs-out) by block the CNT channels. The locations of Au nanoparticles were confirmed by transmission electron microscopy (TEM). Ensemble catalytic activity measurements by UV-vis absorption spectrometer indicated that Au/CNTs-out had the higher catalytic activity than Au/CNTs-in. Single-molecule nanocatalysis experiments were carried out by lab-built prism-type total internal reflection fluorescence microscope (TIRFM) to reveal the location effect between Au/CNTs-in and Au/CNTs-out. The results indicated that Au/CNTs-out was more activity than Au/CNTs-in in reductive N-deoxygenation reaction of resazurin to resorufin. Furthermore, the product molecules on both Au/CNTs-out and Au/CNTs-in preferred the same pathway, reactant-assisted dissociation pathway, but different dissociation rates. The different catalytic performances of Au/CNTs-in and Au/CNTs-out were related to the electron density of Au nanoparticles caused by the its location and nature of CNTs.

Poster Presentation : **ANAL.P-271**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Combined Anion and Nonionic Surfactants-based Micellar Electrokinetic Chromatography with Laser-induced Fluorescence Detection for Quantification of Native Capsaicinoids

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Micellar electrokinetic chromatography (MEKC) equipped with laser-induced fluorescence (LIF) detector was presented for highly sensitive detection of native capsaicinoids. Under running buffer condition of 450 nM Tween 20-15 mM sodium borate-2.2 mM SDS (pH 10), limits of detection (LODs) for capsaicin and dihydrocapsaicin reached 1.3 pM and 3.4 pM, respectively. However, the LODs in UV absorption detection for capsaicin and dihydrocapsaicin was 5.5 nM and 8.1 nM, respectively, demonstrating the presented modality was more sensitive for the capsaicinoids detection. Meanwhile, the mixed micellar surfactants, Twee20-SDS, contributed for improving the separation selectivity and efficiency. In addition, quantification of chili pepper, baechu and kimchi showed 98% confidence indicating there is no significant difference between MEKC-LIF and high-performance liquid chromatography (HPLC). The results demonstrated the developed MEKC-LIF method could provide sensitive on-line detection of capsaicinoids in various foods.

Poster Presentation : **ANAL.P-272**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis, dispersion and tribological performance of alkyl functionalized graphene oxide and graphene-WS2 Composites as an oil lubricant additive

Jong Seok Han, Jin-Yeong Choi, Chang-Seop Lee*

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Graphene and WS₂ 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. GO is 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 First, We have painted a long alkyl chain of graphene oxide (GO) to improve the dispersion of oil-based lubricants with greatly enhanced lipophilicity. Second, a gelator is used for dispersion and a graphene-WS₂ composite is synthesized to improve lubrication performance. 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 (PAO oil) and oil containing WS₂ and also ultrasonicated for dispersion. Graphene-WS₂ composites were synthesized by hydrothermal synthesis, Graphene-WS₂ composites were added to the PAO oil with 1 wt% of the gelator. Chemical and structural properties of the synthesized alkyl functionalized graphene and Graphene-WS₂ composites 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-273**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characteristics and Electrochemical Performance of Graphene/Carbon nanofiber/Silicon Composites as Anode Material for Binder-Free Lithium Secondary Batteries

Ruye Cong, Jin-Yeong Choi, Chang-Seop Lee*

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We report the interfacial study of a Graphene/Carbon nanofiber/Silicon Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon nanofibers (CNFs) were grown via chemical vapor deposition method with an iron-copper catalysts. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 700°C, and maintained for 30 min to synthesize CNFs. GO aqueous dispersion was added into the CNFs/Silicon solution, and the mixture was sonicated for 6h to obtain a GO/CNFs/Silicon aqueous dispersion. Electrode was fabricated by flow-directed vacuum filtration of GO/CNFs/Silicon aqueous dispersion through a filter membrane (90 mm in diameter and 0.22 μm in pore diameter) followed by air drying and peeling off from the filter. The morphologies, compositions and crystal quality of the prepared Graphene/CNFs/Silicon composites were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of Graphene/CNFs/Silicon composites as an anode of Li secondary batteries were investigated using three-electrode cell. The galvanostatic charge-discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester.

Poster Presentation : **ANAL.P-274**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

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

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

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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 OH-doped graphene quantum dots (OH-GQDs) 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. For characterization FTIR, HR-XPS, XRD and electrochemical testing was performed. 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-275**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Control of Different Parameters on Synthesis of Gold Nanorods with High Aspect Ratio

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Seed-mediated method is a general procedure for the synthesis of gold nanorods(Au NRs) who developed Murphy et al. and El-Sayed et al. Many of the interesting optical properties of Au NRs depend on the position of their LSPR peak, which is largely governed by the aspect ratio of Au NRs. However, one of the limitations of the standard seed-mediated procedure is related to the maximum LSPR peak position that can be realistically obtained. So far, previously known LSPR peaks of Au NRs are less than 900nm or more than 1300nm. So, we use hydroquinone as a reducing agent in the presence of silver nitrate to make between range of Au NRs with High aspect ratio. These chemical reagents have an effect on growth of varying length Au NRs. In this study, we have investigated how the change of the reagents in aqueous solution influences on the aspect ratio of Au NRs.

Poster Presentation : **ANAL.P-276**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Proteomics Approach for Plasma Exosomes in Lung Cancer Patients

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Exosomes are cell-derived nanovesicles that are rich source of novel biomarkers in the diagnosis and prognosis of disease. Exosomes have highly-specialized functions and play a key role in processing intercellular signaling. They are present in many complex biological fluids such as plasma. This study intends to identify exosome biomarker from lung cancer plasma. Exosomes were individually extracted from 46 patients' plasma of lung cancer through size-exclusion chromatography. Each exosome sample was pooled into three TNM groups. Each group of exosome samples from lung cancer patients was lysed with RIPA buffer. After Lysis, separated proteins from exosome were trypsin digested. Each group samples were identified nLC-MS/MS using Orbitrap Elite multiple times with various methods for exosomal protein identification from lung cancer plasma.

Poster Presentation : **ANAL.P-277**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A new approach for size determination of nanoparticles by single particle inductively coupled plasma-mass spectrometry (sp-ICP-MS)

Yeon Hee Park, Heung Bin Lim*

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A new approach for the size determination of Au nanoparticles in the size range of 15 nm – 100 nm was explored using single particle inductively coupled plasma-mass spectrometer (sp-ICP-MS). Since current sp-ICP-MS employed aqueous standard solutions to determine the particle size, many assumptions were made and experimental parameters should be determined, which caused measurement errors, although providing universality. In this work, several points were improved to enhance analytical performance in sp-ICP-MS. For higher sensitivity, the level of background subtraction was carefully determined after fitting to a normal distribution, followed by building a correlation curve of average intensity area per particle vs particle radius. When the results were fitted to an allometric function of $Y=aX^3$ at the optimized level of mean plus 3σ , excellent agreement was found, showing a correlation coefficient (R^2) of 0.995

Poster Presentation : **ANAL.P-278**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A resistance study of serum-starvated neuroblastoma cell at specific drug concentration

Sooyeon Chae, Jong Yoon Han, Chae Eun Heo, Min Gyeongseo, MyungKook Son, Min Ji Kim, Hugh I. Kim, Chae Ri Park, Dongjoon Im, Chaehyeon Yoon, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is a solid tumor that arises from the developing sympathetic nervous system. As neuroblastoma belongs to heterogeneous disease, designing effective treatment for each patient is challenging. To examine individual variation in drug response, drug stability and efficiency tests are commonly performed in 2-dimensional (2D) cell or xenograft before clinical trial. However, additional condition to in vitro systems is crucial to closely mimic the complexity of in vivo system. Serum starvation is one of the most frequently used methods to imitate in vivo microenvironment. Thus, examining drug efficacy and resistance of serum-starved 2D cell has been suggested as a screening strategy for individual therapy. However, the differences between serum-starved and normal cells have not been fully understood. In this study, we studied the drug resistance in cancer cell depending on serum starvation. Especially, Topotecan, one of the anticancer drugs which inhibit DNA synthesis, was used. We observed that neuroblastoma cells in serum starvation show the resistance when they are treated with 1 μ M topotecan. Then, quantitation of drug uptake using reverse phase liquid chromatography-triple quadrupole mass spectrometry were performed. As a result of the quantitation of drug uptake, Serum starvation conditions showed relatively lower uptake at 48 hours when chemoresistance occurs. In correlation to distinct change in cellular uptake, we also performed the proteomic analysis to find differentiated protein group related to resistance in serum starvation. The fundamental understanding of anticancer drugs resistance on serum starvation can provide prediction of strategy for individual therapy.

Poster Presentation : **ANAL.P-279**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Measurement of conversion yield of 7-dehydrocholesterol to previtamin D using liquid chromatography-mass spectrometry

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Korea*

Vitamin D is involved in many diseases including sleep disorders, bone metabolism, diabetes, and multiple sclerosis. It is formed from 7-dehydrocholesterol (7-DHC) present in the human skin. When 7-DHC receives UV-B (280-315 nm), it becomes previtamin D and then is converted to vitamin D by thermal isomerization. Herein, we report an analytical method to quantify the conversion yield of vitamin D from 7-DHC by UV irradiation based on liquid chromatography-mass spectrometry (LC-MS), which has a higher selectivity compared with conventional LC-UV. In order to find optimal irradiation conditions, the conversion yields of 7-DHC to previtamin D were measured by varying irradiation time and light source wavelength. After 7-DHC was exposed to a UV-B source in vitro with light intensity of 0.5 mW / cm² for 0-120 sec, 7-DHC, previtamin D, and vitamin D were separated on a Zorbax SB phenyl column and analyzed by a quadrupole-time-of-flight mass analyzer. The conversion yield of 7-DHC to previtamin D increased steadily with increasing irradiation time at all UV-B wavelengths and showed the maximum yield of 10% with UV-B irradiation for 120 sec at 285 nm.

Poster Presentation : **ANAL.P-280**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

High-throughput measurement of lipid turnover rates using 15T FT-ICR mass spectrometry

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Alteration in lipid dynamics is highly associated with various diseases including diabetes and atherosclerosis. Measuring *in vivo* lipid turnover rates at the molecular level can provide insight for better understanding of disease metabolism. The extensive occurrence of isomeric and isobaric lipids is a major bottleneck for studying lipid dynamics on a global scale by mass spectrometry (MS). An ultra-high resolution mass spectrometer is a promising solution to distinguish lipid isobars. In this presentation, we investigated the performance of Fourier Transform-Ion Cyclotron Resonance (FT-ICR) MS in the high-throughput measurement of lipid turnover rates in HeLa cell using partial deuterium oxide (D₂O) labeling. HeLa cells were cultured in 5% (mol/mol) D₂O enriched media and harvested at 8 different labeling times (0, 3, 6, 12, 18, 24, 36, and 48 hr). Lipid extracts from HeLa cell were separated by Ultra-Performance liquid chromatography and analyzed by ultra-high resolution 15T FT-ICR mass spectrometer for differentiation of lipid isobars. High-throughput determination of lipid turnover rates was performed on a global scale by employing our in-house built software. As a result, 424 and 192 lipids were identified at the species level in positive and negative ion mode, respectively. Turnover rates of 48 lipids covering 12 lipid subclasses were obtained in the range 0.0048 to 0.15 hr⁻¹.

Poster Presentation : **ANAL.P-281**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optimization of sample preparation methods for the multi-class chemical analysis of the deciduous teeth

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Exposomics, a research field that tries to measure all the exposures of an individual and reveal how the measured exposures relate to health, receives an increasing attention. Recently, deciduous teeth have been proposed to be retrospective temporal biomarkers for exposomics researches due to its specific structure and growth pattern. However, sample preparation and analysis steps for the tooth matrix have not been explored extensively and need to be standardized. In this study, we evaluated various sample preparation procedures for extracting small organic chemicals from tooth samples and tried to develop a fast and reliable LC-MS/MS method for quantifying multi-class exposure chemicals. With the optimized sample preparation and analysis protocol, various environmental exposure chemicals such as phthalates, phenols, and paraben were quantitatively measured from the deciduous tooth samples.

Poster Presentation : **ANAL.P-282**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Multi-element analysis of deciduous teeth by inductively coupled plasma mass spectrometry (ICP MS)

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Deciduous teeth have a unique characteristic that exposure chemicals accumulated at the prenatal period and at the postnatal period are spatially separated by the neonatal line in their microstructures. Because of this feature, deciduous teeth have been regarded as retrospective temporal biomarkers. In addition, deciduous teeth can provide direct signatures of fetal period exposures whereas other frequently-used biomarkers such as maternal blood, maternal urine, and cord blood can only give indirect ones. In the previous studies, we tried to develop a quantitative elemental analysis method for deciduous teeth by employing a microwave-assisted sample preparation method and inductively coupled plasma dynamic reaction cell mass spectrometry (ICP DRC MS). In this study, we validated a developed method with the bone meal standard reference material and applied a validated method to individual deciduous tooth samples. As a result, concentrations of over ten elements were successfully determined from five individual tooth samples and compared.

Poster Presentation : **ANAL.P-283**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Implementation of LC-MS based proteomic analysis for investigating the tumorigenic roles of PAF in lung adenocarcinoma

Jiwon Hong, Dowoon Nam, Jingi Bae, Seunghoon Back, Su-Jin Kim, Sang-Won Lee*

Department of Chemistry, Korea University, Korea

Lung adenocarcinoma (LUAD) is known to contribute as the most common category in lung cancer. Where proliferating cell nuclear antigen-associated factor (PAF) is associated with cell plasticity, cell stemness, cell hyperproliferation and gene transactivation, it is specifically expressed in tissue stem cells and cancer cells including LUAD. Nonetheless, its role in LUAD still remains to be unclear. Here, we plan to reveal the oncogenic roles of PAF in lung adenocarcinoma employing a comprehensive LC-MS based proteomic analyses on overall protein and phosphorylation changes. With the 6-plex TMT labeled peptides of the control and PAF knockdown cancer cell lines, quantitative profiling of global proteome and phosphoproteome were conducted for both human and mouse samples. Our profiling experiments resulted in identification of 306,938 distinct peptides of 11,689 protein groups and 21,974 distinct phosphopeptides of 17,822 phosphorylation sites for mouse cell lines, and 27,503 distinct peptides of 11,336 protein groups and 21,080 distinct phosphopeptides of 17,461 phosphorylation sites for human cell lines, respectively. From the currently identifying PAF knockdown-induced protein changes, phosphorylation changes and their associated pathways, we aim for a more comprehensive understanding of the pathogenic roles of PAF in the progression of LUAD.

Poster Presentation : **ANAL.P-284**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of extensive global proteome and phosphoproteome profiling platform for effective proteogenomic analysis on human cancer tissue

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Mass spectrometry-based bottom-up proteomics is currently the leading method for large-scale proteome identification and quantification. Importance of proteomics can be highlighted by several aspects such as the lack of coverage that mRNA can precisely predict protein expression. Many of recent proteomic analysis provide increasingly extensive and deep proteome data due to the developments in mass spectrometry of high sensitivity and accuracy, effective fractionation, high-resolution separation and highly informative data analysis method. However, current proteomic data still suffers low in gene coverage compared to genomic data mainly because of the large dynamic range and complex PTMs of a proteome. The large discrepancy in gene coverage of proteomic and genomic data prevents an effective integration of the two data in proteogenomic studies. Here we report a novel dual-online noncontiguous fractionating and concatenating reverse-phase/reverse-phase liquid chromatography (DO-NCFC-RP/RPLC) technology employing online and its application for extensive proteome profiling. When combined with multiplexing capability of TMT and efficient enrichment of “one-pot” IMAC, the platform resulted in significantly improved analysis depth in phosphoproteome.

Poster Presentation : **ANAL.P-285**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Proteogenomic analysis of diffuse-type gastric carcinogenesis induced by E-cadherin, p53, and Smad4 loss in mice

Jingi Bae, Su-Jin Kim, Sang-Won Lee*

Department of Chemistry, Korea University, Korea

Gastric cancer (GC) is the second most common cause of cancer related deaths worldwide, which can be divided into adenocarcinomas of the diffuse and the intestinal type according to the Lauren classification. A recently study reported the establishment of the Pdx-1-Cre;Cdh1^{F/+};Trp53^{F/F};Smad4^{F/F} (pC^{he}PS) mouse model, which spontaneously generates metastatic gastric tumors that closely recapitulate human diffuse-type gastric cancer (DGC). An interesting feature of this model is that the developed DGCs display a near-complete loss of E-cadherin expression (encoded by Cdh1). In order to investigate the functional cooperation of Smad4, p53, and E-cadherin loss in DGC carcinogenesis at the molecular level and to delineate the mechanism of Cdh1 repression, we performed a proteogenomic analysis. In this study, we identified 145,816 peptides and 7,058 unique proteins by using Uniprot DB with MS-GF+ search engine. The in-depth quantitative proteomic analysis identified 1448 differentially expressed proteins ($|\text{DEPs}| \geq 2 \text{ FC}$) in DGCs when compared to normal gastric epithelium (NGE). Through a series of comprehensive proteogenomic analyses of our unique mouse models, we have uncovered important pathways and key mediators involved in DGC carcinogenesis. We suggest promising target molecules in DGC carcinogenesis, including Spp1 and its downstream effector Bcl-xL. Moreover, we identified Tβ4 and Zeb2 as important potential repressors of E-cadherin in DGC carcinogenesis.

Poster Presentation : **ANAL.P-286**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Label-free proteome profiling of ectopic and nonectopic fats related to type 2 diabetes mellitus

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Ectopic fats, such as visceral and pericardial fats, are increasingly recognized as endocrine organs playing important physiological and pathological roles in metabolic abnormalities including obesity, cardiovascular disease, and type 2 diabetes mellitus (T2DM). Despite their pathophysiological importance, proteomes that characterize their functions and are associated with metabolic abnormalities have not been systematically reported. Here, we present comprehensive proteomic analysis of subcutaneous (nonectopic), visceral, and pericardial fats in T2DM patients and subjects with normal glucose tolerance (NGT). A total of 64 tissues of five different tissue types (SAT, VAT, PAT, artery and atheroma) of 16 patients were used for global quantitative proteome profiling. For deep proteome profiling, each of the 4 tissue types (SAT, VAT, PAT, artery) was divided into 24 fractions using mid-pH RPLC fractionation. A total of 288 LC-MS/MS experiments (Triplicate LC-MS/MS experiments of 64 individual samples and 96 LC-MS/MS experiments of mRP fractionation samples) were performed by LTQ-FT Ultra mass spectrometer which was coupled to a dual-online LC system. An extensive profiling generated comprehensive proteome information including 907, 1172, 1716 proteins for subcutaneous, visceral, and pericardial fats, respectively. 738 proteins were commonly detected in all three fat types and 1040 proteins were commonly detected in two ectopic fats (visceral and pericardial). 88 proteins were specifically detected in subcutaneous fats while 97, 630 proteins were specifically detected in visceral and pericardial fats, respectively.

Poster Presentation : **ANAL.P-287**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Integrated Multi-Stage Data Analysis for Next-Generation Cancer Proteogenomics study

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Large-scale cancer genome sequencing studies have generated an extensive catalogue of mutations as disease biomarker and potential therapeutic targets. Difficulty in differentiating the driver and passenger mutations hinders the future development of drug targets hypothesis. Proteins are central to cellular functions, and mutated proteins can drive the initiation of tumor, progression and thereby act as targets to treatment. Proteomics enable an opportunity for functional interpretation of these mutations for better understanding of etiology of cancer development and thence target for therapeutic developments. Proteogenomics provide opportunities for protein level validation of genomic alterations guided by genomics data (RNA-Seq/Exome Seq). More than 300 different types of protein modifications have been described, many of which are known to have pivotal roles in cellular physiology. Protein and their PTM sites is key to dissection of PTM-mediated cellular processes and disease. Here we developed a sensitive method utilizing multi-stage database search for comprehensive proteomics data analysis to complement genomics sequencing data. We employed two complementary search engines, MS-GF+ and MODa/MODi here. The tandem MS data were first subjected to MS-GF+ database search (1st stage search) for mutation search using RNA-Seq guided sample specific mutated proteomics database (generated using CustomProDB) and the unidentified MS/MS data from the 1st stage search were analyzed with the combined use of MODa and MODi (2nd stage search), tools for blind and unrestrictive modification search using the same sample specific mutated proteomics database, respectively. When combined with mPE-MMR, a tool for accurate and extensive precursor masses assignments to co-fragmented MS/MS data, our method was shown to significantly increase the identification of peptides, post-translationally modified (PTMs) peptides, mutated peptides/genes. The developed method will be used for integrated cancer proteogenomic analyses.

Poster Presentation : **ANAL.P-288**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A mitochondrial proteome profile indicative of type 2 diabetes mellitus in skeletal muscles

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The type 2 diabetes (T2DM) is closely related to mitochondrial function in insulin responsive tissues. The mitochondrial proteomes can provide comprehensive information on the function of T2DM-related mitochondria for thousands of mitochondrial proteins compared to the mitochondrial genome, which contains only 37 genes in humans. However, the T2DM-associated protein signatures in insulin-responsive tissues are still unclear. Here we performed extensive proteome profiling of mitochondria isolated from skeletal muscles in T2DM patients (n = 9) and non-diabetic controls (n = 9) to understand the mitochondrial proteome associated with T2DM. We employed filter-aided sample preparation to improve detection of the proteins incorporated in mitochondrial membranes. Furthermore, the use of ultra-high pressure nano-LC-MS/MS coupled with extensive fractionation provided comprehensive mitochondrial proteomes, including 23,122 peptides for 1,150 proteins. Comparison of the mitochondrial proteomes identified 335 differentially expressed proteins (DEPs) between T2DM and non-diabetic samples. Functional and network analysis of the DEPs showed that mitochondrial metabolic process was down-regulated and mitochondria-associated ER membrane (MAM) processes were upregulated. Of the DEPs, we selected two for downregulated oxidative phosphorylation and three for upregulated calcium and protein transport as representative mitochondrial and MAM processes, respectively, and then confirmed their differential expression in independent mouse and human samples. Therefore, we propose that five proteins be used as a potential protein profile that is indicative of the dysregulation of mitochondrial functions in T2DM, representing downregulated oxidative phosphorylation and upregulated MAM functions.

Poster Presentation : **ANAL.P-289**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Parallel Reaction Monitoring to Verify Biomarker Candidates for High-Risk Diabetes Mellitus

Jiwon Ha, Seunghoon Back, Sang-Won Lee*

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Diabetes mellitus (DM) is a worldwide common chronic disease that can cause various complications. If patients of high DM risk were diagnosed in early stage, immediate and suitable treatments can prevent the DM development. Early diagnosis, however, remains difficult due to its symptomless characteristic of DM. Especially, Korean (or Asian) were known to have different patterns of risk factors for DM from those of European so that Korean specific diagnosis method is needed. We performed experiment using DM high-risk patient blood samples which were prospectively collected over past 10 years. We aimed to identify the biomarkers that can predict whether high-risk patients would maintain their condition or develop to DM. Using high resolution 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 C18 column and 200 min LC gradient were used in experiment. Stable isotope labeled (SIL) peptides were used to validate the candidates identified in discovery experiments, resulting in a set of verified candidates for early diagnosis of DM.

Poster Presentation : **ANAL.P-290**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Highly sensitive fluorescent sensor based on novel coordinated amphiphilic polythiophene nanohybrids for triacetone triperoxide explosive detection

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Department of Chemistry, Changwon National University, Korea

Triacetone triperoxide (TATP), one of the most dangerous primary explosives, has emerged as an explosive of choice for terrorists in recent years. A new strategy for the detection of TATP is developed by utilizing amphiphilic polythiophene-coated CdTe QDs (P1QDs) and Hg²⁺ ion. The emission of P1QDs is found to be quenched in the presence of Hg²⁺ ion by electron transfer. Upon addition of the TATP, the quencher (Hg²⁺ ion) has been removed from the surface of P1QDs owing to the strong interactions between TATP and metal ions (Hg²⁺ ion), which leads to significant fluorescence recovery of P1QDs. The detection limit for TATP is 87 µg/L. The simultaneous possession of high sensitivity and selectivity could enable this sensor to be potentially applicable for ultrasensitive and rapid detection trace of TATP in real samples. **Keywords:** amphiphilic polythiophene nanohybrids, metal ions, fluorescence recovery, triacetone triperoxide (TATP), real samples

Poster Presentation : **ANAL.P-291**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mechanism of trinitrophenol explosive detection with novel multiple emitting quantum dots coated with amphiphilic conjugated polythiophenes

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The novel type of multiple emitting CdTe quantum dots (QDs) coated with amphiphilic conjugated polythiophenes has been developed for the determination of the 2,4,6-trinitrophenol (TNP) explosive. Overall, four types of nanohybrids were designed based on the QDs coated with differently charged polythiophenes (cationic, anionic, and nonionic) and thiophene copolymer. The integration of QDs aimed to increase the electron density of polythiophenes which resulted in efficient interaction of the developed nanohybrids with electron-deficient TNP. This was confirmed by considerable fluorescence quenching of the developed sensors when their response to various types of nitroexplosives was studied: nitrophenols and specifically TNP caused the most remarkable fluorescence quenching compared to the other nitroaromatics. Among the developed nanohybrids, positively charged polythiophenes demonstrated the most efficient fluorescence quenching due to the attraction of –OH groups of TNP to the surface of such nanohybrids. The results of time-resolved fluorescence measurements revealed the presence of static quenching through the formation of ground state electrostatic interactions which excludes the excited state energy transfer with Förster resonance energy transfer (FRET) mechanism and suggests the inner filter effect (IFE) as a reason of fluorescence quenching of the sensors. In addition, the contribution of hydrogen bonding, electrostatic, and π - π interactions formed between TNP and QD nanohybrids resulted in high fluorescence quenching of up to 96% as well as in the detection of ultralow amounts of TNP up to 0.56×10^{-9} M.

Poster Presentation : **ANAL.P-292**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of melamine specific bioreceptor using phage-display and their verification

ChanYeong Park, Seung Hoon Back, Tae Jung Park*

Department of Chemistry, Chung-Ang University, Korea

Recently, concerns about safety in food have increased, because carcinogens or illegal hazardous substance are discovered to cheat its component contents. There are many kinds of dangerous reagents, we have investigated the melamine. Originally, it was mostly employed to synthesize melamine-formaldehyde resins, laminates, and plastics. However, some people added the melamine in dairy products. Since the quality evaluation of dairy products is conducted by measuring nitrogen contents. The ingested melamine can crystallize in human renal and induce acute nephrolithiasis and kidney injury. Thus, the detection of melamine is the momentous issue. To detect the melamine, advanced analytical equipment such as liquid and gas chromatography, and Raman spectroscopy were introduced, but they demand for the skilled person, high cost, and long time. Even though the optical detection methods, such as colorimetry and fluorescence, are also being developed as another detection method, it is difficult to specifically detect the melamine since they just recognize the structural features of melamine like aromatic ring or hydrogen bond. In this regard, we have developed specific bioreceptors that selectively bind to the melamine through the phage-display technology. The technique has been used to find out the new bio-receptors for the target such as cell-surface proteins, chemical hapten, etc. In this study, we have discovered melamine-specific binding peptides and evaluated their specificity and affinity against the melamine using graphene oxide quantum dot (GOQD)-Hg²⁺ quenching system. As a result, they showed the high attraction for melamine with a low level of detection limit and appear the probability as a detection sensor for the electrochemical and colorimetric analyses.

Poster Presentation : **ANAL.P-293**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of Novel Upconversion Nanoparticles Functionalized with Amphiphilic Polymers for detection of Alprenolol

Seung Ha Lee, Salah Mahmoud Tawfik Ahmed, Yong-ill Lee*

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Upconversion nanoparticles (UCNPs) are a unique type of photoluminescence(PL) material in which lower energy excitation is converted into higher-energy emission via multi-photon absorption processes. In this research, novel amphiphilic copolymers were synthesized to act as functionalizing agents for NaLuGdF₄:Yb³⁺/Er³⁺ UCNPs. The UCNPs coated with amphiphilic copolymers were characterized by using FTIR, ¹HNMR, SEM, TEM, UV, and PL instruments. These materials were used as optical sensors to detect Alprenolol which is kind of high blood pressure treatment. Our developed sensors displayed good analytical performance such as low limits of detection and good linearity. Furthermore, the sensors were applied to determine the level of high blood pressure drugs in human urine and serum samples with good recoveries. **Keywords:** Upconversion nanoparticles, amphiphilic copolymers, optical sensors, alprenolol, human serum samples, human urine samples

Poster Presentation : **ANAL.P-294**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Detection of C₁₈-ceramide through a novel μ PAD coupled with mass spectrometry

Shavkatjon Azizov, Sharipov Mirkomil, Salah Mahmoud Tawfik Ahmed, Huy B.t., Huy B.t., Yong-ill Lee*

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We developed an innovative wax-printed microfluidic paper-based analytical device (μ PAD) coated with paraffin has been as a highly efficient and low-cost microfluidic device resistant to common mass spectrometry organic solvents. The prepared novel μ PAD-MS system has been introduced for the analysis of C₁₈-ceramide through complexation with metal ions. In contrast to simple paper spray system, the developed μ PAD has allowed the analysis of low concentration of C₁₈-ceramide due to the maximum supply of deposited analyte through a microchannel. The MS results established the formation of doubly and singly charged metal ion complexes between ceramide and different metal ions. Especially, the complexation that occurs between lithium ions and C₁₈-ceramide showed a high relative abundance over other formed complexes. The established μ PAD has shown its prospective in the analysis of hydrophobic biomolecules dissolved in organic solvents and at the same time to avoid their penetration through the developed barriers. The developed μ PAD-MS technique provides clear advantages over the other methods by reducing the number of experimental steps and simplifying the operation process for the identification of C₁₈-ceramide.

Poster Presentation : **ANAL.P-295**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Novel zwitterionic fluorescent polythiophene sensor for E.coli. detection

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We developed a novel zwitterionic fluorescent polythiophene with high sensitivity for the detection of gram-negative pathogenic bacteria. The sensing probe using the zwitterionic fluorescent polymer was constructed with three different water soluble thiophene monomers via oxidative polymerization reaction. The zwitterionic fluorescent polythiophene bound to bacteria through ionic complexes between anionic groups on the bacterial surface and cationic groups after 15 min incubation. This finding demonstrated that the fluorescence on system operated via changes in the hydrophilic and hydrophobic nature of the zwitterionic fluorescent polymer at pH (7.4), at a fixed polymer concentration. The limit of detection for *Escherichia coli* was found to be 0.033 cfu/mL with linear range from 1.15×10^8 - 1.15×10^9 cfu/mL. With these encouraging results, it is expected that it would open revenues for promising applications of zwitterionic polythiophene in real samples. **Keywords** : zwitterionic polythiophene, Gram-negative bacteria, E.coli, Fluorescence enhancement, Bacterial surface

Poster Presentation : **ANAL.P-296**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

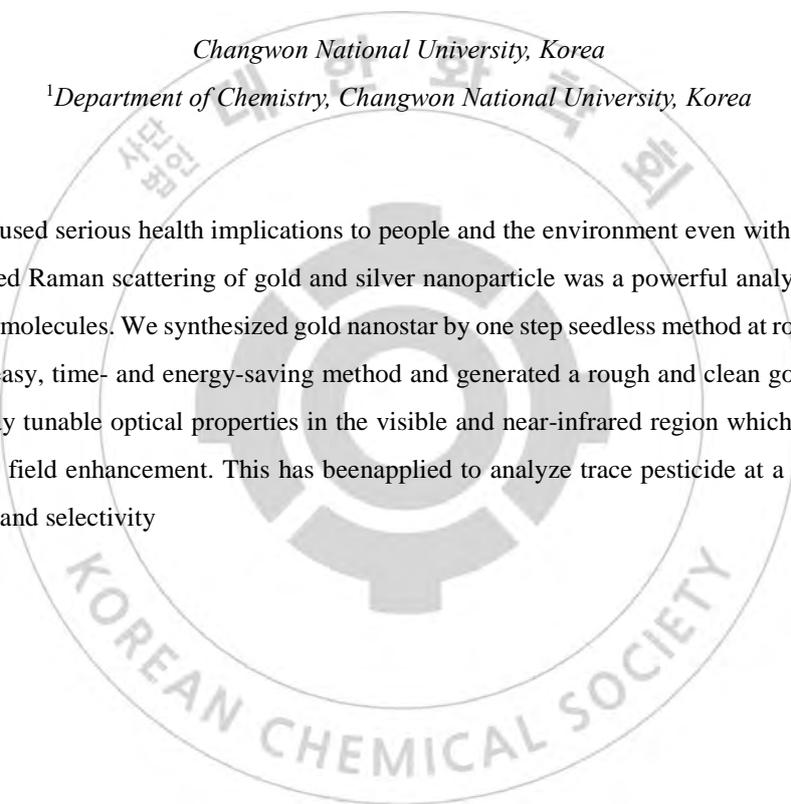
Gold nanostar-based SERS substrate for pesticide analysis

Hung Thai viet, Huy B.t.¹, Yong-ill Lee^{1,*}

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Pesticide has caused serious health implications to people and the environment even with a small amount. Surface-enhanced Raman scattering of gold and silver nanoparticle was a powerful analytical tool for the sensing of trace molecules. We synthesized gold nanostar by one step seedless method at room temperature. This method is easy, time- and energy-saving method and generated a rough and clean gold surface. Gold nanostars display tunable optical properties in the visible and near-infrared region which lead to a strong electromagnetic field enhancement. This has been applied to analyze trace pesticide at a small scale with high sensitivity and selectivity



Poster Presentation : **ANAL.P-297**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Nonionic alginate-coated upconversion nanoparticles functionalized with folic acid for selective NIR-imaging and pH-responsive drug delivery

Sharipov Mirkomil, Salah Mahmoud Tawfik Ahmed, Huy B.t., Yong-ill Lee*

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Rare-earth upconversion nanoparticles (UCNPs) have been proposed as biological luminescent labels for the bioimaging application of future because of their property to convert NIR irradiation to visible light. However, their toxicity, low dispersion, and low selectivity call into question their suitability in nanomedicine. To address these challenges, naturally modified nonionic alginate-based polymers were successfully synthesized and coated onto upconversion nanoparticles (UCNPs) to act as functionalizing agents. The developed hybrid polymer-UCNPs nanoparticles have showed a high stability and excellent biocompatibility. These hybrid nanoparticles have shown a selective NIR imaging of KB cells due to the presence of folic acid. Moreover, the presence of large cavities of materials and amphiphilic polymer shell, these hybrid nanoparticles were able to efficiently load the anticancer drug doxorubicin (DOX) as well as to release it in highly controlled and selective manner via folate receptor-mediated endocytosis. Cytotoxicity test against KB cells have confirmed that hybrid nanoparticles loaded with DOX have a higher inhibition of growth of KB cells compared to free DOX. The developed theranostics platform is capable to simultaneously perform imaging and deliver anticancer drugs and thereby is expected to grant a valuable innovation in bioimaging and nanomedicinal applications.

Poster Presentation : **ANAL.P-298**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Graphene oxide as a peroxidase mimetic catalyst for detection of Cr(VI) ions

Nguyen Ngoc Nghia, Huy B.t.¹, Yong-ill Lee^{1,*}

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Graphene oxide (GO) was used as a peroxidase mimetic catalyst to detect hexavalent chromium (Cr(VI)) in aqueous solutions. The color change of tetramethyl benzidine (TMB) which was catalyzed by GO. The color of the probe will be turned "OFF" and "ON" by adding 8-hydroxyquinoline (8-HQ) and Cr(VI), respectively. The mechanism could be explained due to the chelation reaction between 8-HQ and Cr(VI). The color change can be observed by naked eyes or UV-vis spectrophotometer. Under the optimal experimental conditions, the prepared probe exhibited high selectivity, limit of detection (6 nM), and large linear range. This study was applied successfully for Cr(VI) detection in real water. Keywords: hexavalent chromium; chelate; graphene oxide; mimetic catalyst; naked eyes.

Poster Presentation : **ANAL.P-299**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Picogram detection of nitro-explosive compound using multiple emitting Polythiophenes-Coated CdTe QDs

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A facile in-situ polymerization strategy has been performed to synthesize novel multiple emitting amphiphilic conjugated polythiophene-coated CdTe quantum dots as an optical sensor for the rapid, sensitive, selective, and on-site detection of 2,4,6-trinitrophenol (TNP). More importantly, portable, disposable, cost-effective, and easy-to-use paper strips and chitosan film were successfully applied to visually detect TNP concentrations as low as 1 nM. Using a smartphone with an easy-to-access and color-scanning App as a detection platform for the quantitative determination of TNP has also been demonstrated. The quantum dot-based sensor not only exhibits an excellent selectivity for TNP comparing with its analogues, but also possesses an excellent limit of detection of 0.56 nmol L⁻¹ with linear ranges of 0.05-14 μmol L⁻¹. Furthermore, the quantum dot 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 1.54-2.32% and 1.44-2.81%, respectively. This work unveiled an effective method for the sensitive and selective detection of TNP explosive toward national security and environmental protection. **Keywords:** QDs, trinitrophenol (TNP), river water, electron transfer mechanism.

Poster Presentation : **ANAL.P-300**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

New Ru(ter-py)(dmo-bpy)Cl redox complex for glucose dehydrogenase based glucose biosensor

Ryang hyeon Kim, Hyewon Jang, Subin Park, Won-Yong Jeon, Young Bong Choi*, Hyug-Han Kim*

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Unlike the central metals Os and Fe, which have been studied extensively, we synthesized new mediator using the same Group 8 element Ru. In this study, we used 2,2'-6',2''-terpyridine (ter-py) and 4,4'-dimethoxy-2,2'-bipyridine (dmo-bpy) as a ligand used for glucose sensor. The electrochemical property of the synthesized Ru(ter-py)(dmo-bpy)Cl complex was confirmed by cyclic voltammetry (CV). Conventional glucose sensor has measured the concentration of the glucose using glucose oxidase (GOx) enzyme, which is affected by the concentration of oxygen in the body. As a result, GOx based glucose sensor has been showed a little bit error due to different oxygen concentration. To solve this problem, we have fabricated glucose sensor electrode using glucose dehydrogenase (GDH) and our mediator. The modified glucose sensor electrode transferred the electron from the active site of the enzyme to the electrode efficiency. Also, it has high selectivity and sensitivity, which helps to detect glucose. Our mediator showed possibility for applying to glucose sensor.

Poster Presentation : **ANAL.P-301**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Advanced studies of antibiotic peptides using solid-state NMR

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The important of adequate amounts antibiotic use can't be overestimated. Due to the abuse of classical antibiotics, antibiotic resistance has been increasing. So studies of cationic amphipathic peptides come into the spotlight as a new antibiotic. And there is still the potential for being used as candidate of good antimicrobial agent. It is also indispensable to discover new compounds to counteract the existing antibiotic resistant bacteria in the world. Lactophorin is a cationic amphipathic peptide with 23-amino acid residues derived from bovine milk. And we developed another new design to develop other novel AMPs with a more effective and less toxic antimicrobial using the sequence of the LPcin-YK3 peptide. Antimicrobial activity of designed novel AMP analogs was confirmed by bacterial killing assays and growth inhibition assays for bacteria and fungi, and the stability was confirmed by hemolysis assay and cytotoxicity assay for mouse and human eukaryotic cells. In order to understand the relationship between antibiotic function and structure of AMPs we conducted structural studies of novel AMPs using various spectroscopic methods and NMR. We successfully expressed of LPcin in *E. coli* and purified from the cell extract using various biophysical techniques. To confirm their 3D structures in membrane environments, we conducted solid-state NMR.

Poster Presentation : **ANAL.P-302**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Classification and spectral characteristics of chemical agents by using a deep UV stand-off Raman spectroscopy

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Agency for Defense Development, Korea

Chemical agents (CAs) are highly toxic to human health. It is required to rapidly detect and warn the released CAs to protect human life. The primary contamination of CAs due to attacks occurs mostly on the ground surface, and Raman spectroscopy can quickly identify CAs on the surface in a non-contact manner. In this presentation, we shows the Raman spectra of toxic chemicals including CAs measured by using a Raman spectroscopic system having 248 nm deep UV light source, spectral characteristics of them, and principle component analysis result. From this results, we confirmed that deep UV stand-off Raman spectroscopy could be a potential method for quickly and accurately detecting and classifying CAs contamination.



Poster Presentation : **ANAL.P-303**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

NMR structural studies of mutations in transmembrane proteins related with human diseases

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Human transmembrane proteins (hTMPs) perform essential role like gateway to permit the transport of specific substances. Additionally channel formation, cell-to-cell communication and signal transductions are also important tasks of hTMPs. The starting point for understanding and studying the specific biochemical processes of hTMPs is to determine their three-dimensional structure. The study of the structure of these membrane proteins has been extensively studied because it forms the foundation for new drugs development. The first is the transmembrane domain of amyloid precursor proteins (APP-TM) related Alzheimer's disease. What we pay attention to is the formation of amyloid channels that cause side effects such as and abnormal increase in intracellular calcium concentration. In other words, APP-TM forms a Ca²⁺ permeable ion channel in the cell membrane, destroying calcium homeostasis in normal cells, and such amyloid channels are also found in other amyloidogenic disease-related proteins such as prions and α -synuclein. The next is Syndecan-4 (Syd4), which is involved in signal transduction and cancer progression. They may affect tissue development and repair and grow factors as well as the pathogenesis of numerous diseases, especially such as cancer. The main process of action mechanism of Syd4 is the signal transmission through structural changes by ligand binding, so it is important to examine the three-dimensional structure in order to understand this process. High-purity protein samples obtained from optimized expression and purification processes have been characterized using various analytical techniques and are undergoing structural studies using solution/ solid-state NMR spectroscopy and computer modeling.

Poster Presentation : **ANAL.P-304**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Thermal Decomposition Behavior of Explosives by Accelerating Rate Calorimeter (ARC)

Hae-Wook Yoo, So Jung Lee, Kuktae Kwon, SeungHee Kim*

Agency for Defense Development, Korea

The thermal decomposition behaviors are highly important for hazardous substances since they can be placed in an uncontrollable state through the self-decomposition process. If self-decomposition process is triggered by hazardous material, a significant disaster can occur as process size and stocks increase. Therefore it is essential to analyze thermal decomposition behavior in order to maintain and handle thermal-sensitive materials in a safe state. Among the various hazardous materials, explosives are highly critical in handling and storage issue. In this study, the thermal decomposition behavior of representative explosives, e.g. several particle sizes of RDXs are analyzed, which can provide the guideline for transportation and storage of explosives.

Poster Presentation : **ANAL.P-305**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Analysis of Quaternary Ammonium Compounds (QACs) by Liquid Chromatography-Mass Spectrometry

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After the humidifier disinfectant sacrificed many lives, there has been a growing concern regarding the biocidal chemicals contained in the consumer products we use. Since then, to effectively regulate the chemicals in the consumer products, the Ministry of Environment have begun to strengthen the regulations on the usage of biocides in the consumer products. One of the widely-known biocidal chemicals in commercial products are quaternary ammonium compounds (QACs). QACs are a group of chemicals having a structure of NR_4^+ , positively charged nitrogen atom with four alkyl chains covalently connected to it. Although QACs are extensively used in consumer product, such as a fabric softener, how to evaluate their exposure coefficient and toxicity has not been systematically established. In this research, we developed and optimized an analytical method using liquid chromatography tandem mass spectrometry (LC-MS/MS) for the identification and quantification of 3 different QACs standards like benzylalkyldimethylethylammonium (BAC), alkyltrimethylammonium (ATMAC) and dialkyldimethylammonium (DADMAC). Also isotope substituted QACs were used for relative quantification of targeted materials in the sample. By adopting the method, those compounds were simultaneously analyzed in less than 10 minutes, and linearity, selectivity, accuracy, and precision of the method were evaluated as well. We plan to identify and accurately quantify QACs contained in various commercial products by applying established analytical method.

Poster Presentation : **ANAL.P-306**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Nano-DESI mass spectrometry (MS) source-coupled digital microfluidics system

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Electrowetting on a dielectric (EWOD) digital microfluidics (DMF) is a technology that deals with microscale droplets on the two-dimensional plate in the discrete manner. It has some advantages compared to conventional microfluidics, such as minimal contamination, and simultaneous control of multiple droplets. Because of its simplicity and compatibility, DMF was applied to the various fields as a tool for sample preparation in chemical and enzymatic reactions, immunoassays, DNA-based applications, clinical diagnostics, proteomics, and cell-based applications. A variety of researches about coupling DMF with different detection methods have been also studied including optical, electrochemical, and mass spectrometric detection. In this research, a new coupling platform of DMF/nano-DESI/MS was investigated for proteomics studies. At a glance, the coupling of DMF and nano-DESI is very natural in the quantitative and geometrical manner because both systems deal with microscale samples on the two dimensional plate. Using the DMF/nano-DESI platform, a couple of proteins were enzymatically digested on the DMF chip and the prepared peptides were detected using nano-DESI source. The detailed setup and results will be demonstrated in the symposium.

Poster Presentation : **ANAL.P-307**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Toward the construction of the hazardous accident site gas database using a TD-GC/MS method

Eun Woo Choi, Han Bin Oh*

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In the accident site, for example, fire and terror, the detection of gases remaining in the site may provide some evidence for the accidents. These gases can be used as markers to find how the accident occurred. For this purpose, we are developing a thermal desorption-gas chromatography mass spectrometry (TD-GC/MS)-based method that can provide fingerprints of the accidents. Collection of the hazardous gas fingerprints can provide us with data and eventually it will be expanded into the hazardous accident site gas database. As a showcase, we present two specific TD-GC/MS results obtained in two fire sites in the Great Seoul metro areas. The examples show that TD-GC/MS data may provide some fingerprint in the fire sites and this approach will be expanded in the future to construct the accident site hazardous gas database.

Poster Presentation : **ANAL.P-308**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Free radical initiated backbone dissociation of peptides conjugated with p-TEMPO-Benzyl Succinic Acid

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4-(2,2,6,6-Tetramethylpiperidin-1-oxyl)methyl benzyl succinic acid N-hydroxysuccinimide, so called p-TEMPO-Bz-Sc-NHS, is a newly designed peptide-conjugating reagent for free radical-initiated peptide sequencing (FRIPS) that exhibits improved conjugation efficiency with targeted peptides as compared with previously designed conjugation reagent, o-TEMPO-Bz-radical initiator. p-TEMPO-BZ-Sc-NHS achieves the FRIPS with higher energy collision induced dissociation (CID), which eventually enables the one step MS3 to elucidate the peptide fragmentation. p-TEMPO-Bz-Sc-NHS was conjugated with model peptides and conjugated peptides were analyzed by MS/MS and MS3 to verify the FRIPS on positive ion-mode. One-step CID enabled the C-O cleavage of p-TEMPO-Bz-Sc-C(O)-peptides and dissociated the conjugated peptide complex into p-TEMPO radical and •Bz-Sc-peptide radical. Successive beta hydrogen (H β) extraction of peptide backbone and radical migration dissociated the peptide backbone and produced fragment ions consisting mainly of a-, c-, x-, and z-type ions and those produced from neutral loss. The energetic interpretation of p-TEMPO-Bz-Sc-C(O)-peptides were presented in the form of survival fraction to investigate the energetic dissociation of p-TEMPO. Also, LC-MS analysis was conducted on the mixture of model peptides to see if this p-TEMPO radical initiator could be applied to FRIPS of digested protein in our future research.

Poster Presentation : **ANAL.P-309**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Developing Gas Mixing System for Preparing Standardized Gas Mixture to Properly Analyze Toxic Gases Generated from the Fire

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As the fire occurs, various kinds of toxic gases are generated and different material generates different toxic chemicals. During the investigation of the fire, investigators are easily exposed to toxic gases for a long time. Due to the lack of methodology or instruments enabling the real-time identification of toxic gases present in the field, respiratory-related industrial accidents of on-site police officers are constantly occurring every year. Related government departments have been developing a portable sensor capable of identifying and measuring the amount of poisonous gas in the field so that it can be used to prevent investigators from being exposed to hazardous environments. To test the accuracy and efficiency of the device, we are currently developing of a gas mixing system which is designed to provide standard fire-hazardous gases. The system is equipped with a mass flow controller (MFC) that enables the precise control of the amount of flow and a vacuum gauge that accurately measures gas pressure in the order of a few mtorr. Developed device is expected to allow a reproducible production of standard gases. Accuracy of the concentration of standard gas prepared by developed samples will be evaluated by GC analysis in the future.

Poster Presentation : **ANAL.P-310**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Simultaneous quantitative analysis of a large number of VOCs with a multitude of isotope-labelled internal standards using a headspace GC-MS

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Volatile organic compounds (VOCs) are organic compounds with a high vapor pressure at room temperature. VOCs are often included in a variety of commercial products, such as daily life chemicals, packaging materials, building materials, and soils with purpose. As the VOCs and the matrix material contained in the commercial products are very diverse, it is required to develop a simultaneous quantitative analytical methodology that enables one to accurately and reproducibly measure the targeted VOCs in the products of interest. Toward this goal, a headspace-GC/MS was used to perform a simultaneous quantitative analysis of 26 VOCs by spiking a number of isotope-labelled internal standards. A total of 26 compounds were classified by their structure and physicochemical properties, and six internal standards were utilized. This approach with the isotope-labelled internal standards is expected to overcome the so-called "Raoult's law pitfall of the headspace GC analysis". In this study, the mixture was diluted to five different concentrations to construct a calibration curve for each type of VOCs. In order to quantitatively analyze VOCs contained in the commercial products, the VOC mixture was spiked into five different products. The recovery of targeted materials was made to investigate the correlation between the internal standard and each substance, and the degree of sensitivity relative to the matrix material was evaluated as well to evaluate accurate and reproducible analysis.

Poster Presentation : **ANAL.P-311**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Practical purification methods to obtain human melanocortin-4 receptor related to obesity for structural studies using NMR spectroscopy

Minseon Kim, Ji-Ho Jeong*, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

The human melanocortin-4 receptor (hMC4R), one of human transmembrane proteins (hTMPs), is valuable because they play important role in food intake and energy homeostasis. Therefore, it is hMC4R related in genetic reasons of eating disorder and severe human obesity. The heterozygous mutations of hMC4R, substitute of the 90th amino acid, aspartic acid to asparagine (D90N) located second transmembrane domain (TM2), was found in the patients with early onset obesity. Mutant D90N hMC4R TM2 (m-hMC4R-TM2) is expressed on the cell surface and binds to the ligand with affinity like wild type hMC4R TM2 (wt-hMC4R-TM2), but mutation in MC4R gene decreases MC4R signaling and cAMP content. We thought that structural change of wt-hMC4R-TM2 causing functional loss of m-hMC4R-TM2. In order to examine structural differences of wt/m-hMC4R-TM2 protein, it is important to obtain high yield and high purity of expressed proteins. However, the innate insolubility of transmembrane proteins, it is seriously difficult and time-consuming to prepare the sample of target transmembrane protein. In this research, we demonstrate the optimization and purification procedures to obtain higher yield of wt/m-hMC4R-TM2 proteins for structural studies. In the experimental process, sodium dodecyl sulfate (SDS) was used in FPLC as a detergent because hydrophobicity of target proteins was applied to separate the target transmembrane proteins from impurities. After removing SDS, the obtained wt/m-hMC4R-TM2 proteins were applied to various spectroscopic methods such as MS, CD, solution NMR spectroscopy, and solid-state NMR spectroscopy.

Poster Presentation : **ANAL.P-312**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Automated cold volume calibration of temperature variation in cryogenic hydrogen isotope sorption isotherm

Jaewoo Park, Minji Jung, Hyunchul Oh^{1,*}

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The gas adsorption isotherm requires accurate measurement for the analysis of porous materials which is used as an index of surface area, pore distribution, adsorption amount of gas. Basically, adsorption isotherms of porous materials were measured conventionally at 77K and 87K using liquid nitrogen and liquid argon. The cold volume calibration in such conventional way was simply done by splitting into two zone (cold and warm volume) through controlling level sensor in Dewar filled with liquid nitrogen or argon. As a result, the BET measurement for textural properties is mainly limited to the N₂ or Ar gas. In order to investigate the other gases at various temperature independently, a novel temperature control system for sample cell is required, and consequently the cold volume calibration at various temperature become more important. In this study, the cryocooler system is newly installed in commercial BET device for controlling the sample cell temperature, the automated cold volume calibration of temperature variation for various gases (e.g. hydrogen isotopes) is introduced. This developed calibration method presents reliability and reproducibility of the cryogenic measurements of hydrogen isotope separation in porous materials, and also provide the large flexibility for performing various other gases with temperature.

Poster Presentation : **ANAL.P-313**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Oligomerization of tau protein mediated by electrostatic interaction with ATP

**Jong yoon Han, Chae Eun Heo, MyungKook Son, Dongjoon Im, Gyeongseo Min, Sooyeon
Chae, Chae Ri Park, Min Ji Kim, Paul Valery Migisha Ntwali , Hugh I. Kim***

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The fibrillation of tau, a microtubule-binding protein, in neuron is a hallmark of Alzheimer's Disease. Although the detailed fibrillation mechanism of tau is not revealed, negatively charged biomolecules are considered as crucial factors which can induce tau fibrillation. Adenosine triphosphate (ATP) is an abundant anionic biomolecule with high charge density (1-10 mM in cytosol) and was recently suggested as a potential cause of tau fibrillation. In this study, we investigated the influence of ATP on the structural transition of tau K18 (a four-repeat domain crucial for tau fibrillation) using ion mobility mass spectrometry (IM-MS) and small angle x-ray scattering (SAXS). Our results imply that the ATP induces monomeric K18 to form dimers with the formation of partially folded structure. Overall, our study would be valuable for characterizing the role of ATP as a promoter to induce tau oligomerization in the early stage of fibrillation.

Poster Presentation : **ANAL.P-314**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solution state structure of the mimetic Apo B-100 peptides(B) derived from immunoglobulin antigen by NMR

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Apolipoprotein (apo) B-100 is the major protein found in low density lipoprotein (LDL), which is composed of 4536 amino acids. As cholesterol-transporting lipoprotein in human plasma, Apo B-100 is the ligand that is responsible for the binding of LDL to the LDL receptor. The modification of amino acid residues in apo B-100 by acetylation or malondialdehyde(MDA)-modification interfere with 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 lesion. For this reason, apo B-100 has been given a clinical attention to use of diagnosis marker of atherosclerosis. In this study, a combination of sequence 20, each one named P1-P302 and MDA oxidation treatment. Based on leading research results of increase antibody to recognize oxidized LDL, Atherosclerosis causes likely Apo B-100, Peptide has the characteristics are shown high levels of Immunoglobulin antibodies and MDA process. Homonuclear related two-dimensional NMR experiments techniques COSY, TOCSY, NOESY was used to analyze the complete NMR signal and it was determined by obtaining the 'H-H' distance information to the liquid structure within the peptide sequence through NOESY. 3D NMR structure created using the distance geometry and molecular dynamics method by comparing the values obtained through NOE experimental and 2D NOE back-calculation.

Poster Presentation : **ANAL.P-315**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solution state structure of the mimetic Apo B-100 peptides(A) derived from immunoglobulin antigen by NMR

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Apolipoprotein B-100 (Apo B-100), the major component of low density lipoprotein (LDL), consisting of 4,536 amino acids and these amino acids are classified into peptide group P1-P302 with sequent 20 amino acids. Apo B-100, a lipoprotein that carries cholesterol in human plasma, is responsible for the binding of LDL and LDL receptor. Modification of lysine residues of apo B-100 by acetylation or MDA(malondialdehyde)-modification prevents the binding of LDL and 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. In this study, a combination of sequence 20, each one named P1-P302 and MDA oxidation treatment. Based on leading research results of increase antibody to recognize oxidized LDL, Atherosclerosis causes likely Apo B-100, these peptides has the characteristics are shown high levels of immunoglobulin antibodies and MDA process. Homonuclear related two-dimensional NMR experiments techniques COSY, TOCSY, NOESY was used to analyze the complete NMR signal and it was determined by obtaining the 'H-H' distance information to the solution structure within the peptide sequence through NOESY. 3D NMR structure created using the distance geometry and molecular dynamics method by comparing the values obtained through NOE experimental and 2D NOE back-calculation.

Poster Presentation : **ANAL.P-316**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Graphene Oxide based fluorescent nano-sensor for miRNA with high specificity

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MicroRNAs (miRNAs) is short non-coding RNAs which have emerged as promising next-generation biomarkers in clinical diagnostics. Here, we developed graphene oxide (GO) based fluorescent nano-sensor for miRNA with high specificity and sensitivity. GO, water soluble derivative of graphene, is one of the most popular nanomaterials in bio-medical field over the last few decades. Common strategies of GO based sensors depends on the fluorescence quenching capability of GO and strong adsorption of ssDNA probes on GO surface through pi-pi interaction or hydrogen bonding. Unfortunately, the interaction between DNA and GO is easily interrupted by other molecules in biological sample such as proteins, lipids and nucleic acids, resulting in the nonspecific desorption of probes. Therefore, we designed new duplex probe for miRNA and attached the probes on GO by covalent coupling with carboxylic acid groups of GO, instead of nonspecific adsorption. The probes can bind with target miRNA sequence-specifically, followed by recovering the fluorescent signal. This platform shows improved signal to noise ratio with detection limit at the pico-molar levels. We believe that this new GO based sensor can be a suitable tool for miRNA-based practical diagnostics of diseases providing a valuable resource for basic and applied research.

Poster Presentation : **ANAL.P-317**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and characterization of magnetic-viral Janus nanoparticles

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Janus nanoparticles (JNPs) are unique building blocks which have asymmetric structures. Typical silver nanoparticles which are spherical shapes, for example, are composed of silver themselves and surface is homogeneous. However, JNPs are formed by heterogeneous surface; half of side is different from another side. They have been attracted and studied because of their different chemical or physical properties. For instance, their asymmetry give chiral properties. When we synthesis JNPs using magnetic nanoparticles (MNPs), they are able to be arrayed in magnetic field. Asymmetry and magnetic properties offer efficient and distinctive methods to target complex self-assembled materials. Here, we made Janus magnetic nanoparticles with Fe₃O₄. We coated half of surface with gold through sputtering followed by coordination of M13 bacteriophages and made them be arrayed by magnetic field. JNPs we made seem shuttlecock shapes. To figure out optical properties of nanochains, UV-vis spectroscopy, Raman spectroscopy, and Fourier transform infrared spectroscopy (FTIR) are used. The unique optical properties of suprastructures of JNPs can be applied into color sensors, biosensors, and display research fields.

Poster Presentation : **ANAL.P-318**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Chemiluminescent probes-based 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 each year. Traditional diagnosis methods require high cost equipment and technician for diagnosis of influenza virus. Last decade, the development of alternative diagnosis techniques for influenza has received a tremendous attention of scientist. The emerging paper-based analytical devices (μ PAD) has shown their potential as low cost and easy to use method in 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 fluorescent probe or chemiluminescent is promising in development of novel, low-cost and easy to operate sensing material. 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 chemiluminescent derivative-based μ PAD that is selectively activated in the presence of influenza virus. μ PAD was designed via stacked system to ensure to deliver the influenza virus to the target area after deposition onto μ PAD.

Poster Presentation : **ANAL.P-319**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Ag@Fe₃O₄ nanoparticles with chiral ligands

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Chirality is a property of asymmetry that has a non-superposable mirror image. The notable property of chirality is the enantioselectivity that is observed in organic, biochemical reactions. It has two forms, L-, D- forms. In some cases, one form is used for medicine, however, the other form has a nonmedical or toxic. So recent developments are focused on this importance to separate two forms by chiral materials. Additionally, by using chiral nanostructure it is possible to controlling polarization of the light. To develop nanoparticles with higher enantioselectivity and polarization selectivity, chiral nanoparticles were synthesized by adsorbing chiral molecules on its surface. Ag@Fe₃O₄ nanoparticles (NPs) are achiral materials and because of the composition of the shell of the iron, it has a magneto-plasmonic (Mag-plas) property that can be assembled and regulated outer magnetic field and enhanced with varying the shell porosity via an etching process. With increasing shell porosity, the Ag@Fe₃O₄ NPs are modified to produce highly enhancement of the catalytic activity and surface-enhanced Raman spectroscopy (SERS) effect, resulting from enhanced chemical diffusion into the Ag core. By adsorbing ligands on the surface, we tried to develop Ag@Fe₃O₄ NPs with chiral surface. Moreover, we tried to modify inner structure by using chiral molecules while crystal formation process of NPs. With this chiral magneto-plasmonic it can be possible to use in biochemistry to distinguish opposite chirality with higher selectivity, which can be used as biosensor and catalyst.

Poster Presentation : **ANAL.P-320**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

SERS-based microdroplet system for high-throughput gradient analysis

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Microfluidic technology has emerged as a highly efficient tool for the study of various chemical and biological reactions in last two decades. Recently, we reported that high-throughput biomarker detections can be achieved using a single phase gradient microfluidic channels together with surface-enhanced Raman scattering (SERS) detection. However, the deposition of nanoparticle aggregates on channel surfaces induces the “memory effect” in the continuous flow regime, thus affecting both sensitivity and reproducibility. To resolve this problem, a SERS-based gradient microdroplet system has been developed in this work. Herein, the sample stacking problem could be solved since two-phase liquid/liquid segmented flow reduces the memory effect. A serial dilution of a reagent could be also achieved in a stepwise manner using microfluidic concentration gradient generators. Therefore, desired concentrations of a reagent could be sequentially trapped by a small volume of droplets to prevent the sample stacking. We believe that this microdroplet system will be of significant utility in monitoring chemical and biological reactions for various concentrations of a reagent.

Poster Presentation : **ANAL.P-321**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication of PEGylated Au@Ag core-shell nanoparticles for SERS imaging of multiple biomarkers expressed on cancer cells

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Implementation of the use of metal nanoparticles in cellular imaging has been recently garnered much attention. We recently developed a surface-enhanced Raman scattering (SERS)-based cellular imaging technique to detect cancer phenotype markers expressed on cell surfaces. Therein, hollow gold nanospheres (HGNs) have been used as SERS nano tags since HGNs strongly enhance the Raman signal intensity of individual nanoparticles by localized surface plasmon effects through the pin holes in the particle structures. However, this technique has some limitations including desorption of Raman reporter molecules and aggregation of HGNs in aqueous condition. To resolve these problems, polyethylene glycol (PEG)-ylated silver shell-gold hollow core nanoparticles (AgHGNs) have been fabricated and used as SERS nanotags in this work. By the silver shell encapsulation, the desorption problem of Raman reporter molecules could be solved. In addition, the SERS intensity of AgHGNs was greatly enhanced over HGNs. Then these particles were encapsulated with PEGs to make them stable in different pH, temperature and salt conditions. Finally, these PEGylated AgHGNs were used for the SERS imaging of three different tumor-associated biomarkers (CD44, EpCAM and ErbB2) expressed on breast cancer cells to confirm their multiple marker detection capability.

Poster Presentation : **ANAL.P-322**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Highly sensitive molecular diagnostics using SERS-PCR for Bacillus anthracis detection

Yixuan Wu, Younju Joung, Sohyun Park, Jaebum Choo*

Department of Chemistry, Chung-Ang University, China

The real-time polymerase chain reaction (QPCR) technique has been extensively used for the diagnosis of a wide range of infectious diseases. This technique found valuable clinical applications in the diagnosis of viral diseases but it suffers from several problems including time-consuming process and high fluorescent background noise. To resolve these problems, we developed a conceptually new surface-enhanced Raman scattering (SERS)-based PCR technique for its clinical applications. Due to its highly sensitive detection capability, it was possible to determine the concentration of target DNA in a short time by decreasing the number of PCR cycles. Consequently, SERS-PCR provides a high sensitivity and a short detection time over the conventional fluorescence-based QPCR. In the present study, we employed TaqMan-PCR to amplify a target gene, and then used the SERS detection technique for its highly sensitive detection. The combination of PCR with SERS proves to be effective for the rapid and sensitive detection of a low concentration of a target gene in a short time.

Poster Presentation : **ANAL.P-323**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Metabolomic analysis of human blood associated with ambient particulate matter in air pollution

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Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Korea

Ambient particulate matter (PM) has become the major environmental risk factors in Korea, and exposure to PM is associated with adverse health effects on human. The objective of this study was to assess the alteration in response to environmental exposure and to investigate the association between levels of metabolite identified in human whole blood samples and PM with a diameter 2.5-10 μm (PM10).

In this study, we analyzed human whole blood from 457 Koreans using ^1H -NMR spectroscopy. The concentration of PM10 was used in multivariate linear regression model adjusted for age, sex, BMI, and smoking status. We found that PM10 was significantly related to energy metabolism such as lactate, pyruvate, glucose, and fumarate.

This approach can be a novel tool to identify potential biomarkers for predicting exposure of pollutants like PM10 and to assess the impacts of environmental pollution on human metabolism.

Poster Presentation : **ANAL.P-324**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Metabolic profiling of plasma and urine from a randomized trial on the effects of dietary patterns.

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Korea Basic Science Institute, Korea

¹Department of Chemistry, Sungkyunkwan University, Korea

Habitual diet plays an important role in the metabolic profile and composition of the gut microbiota that can affect the host. To investigate the potential benefits of the Korean diet which is plant-based diet compared to western diet, we analyzed the changes of metabolites and gut microbiota after Korean diet (KD), the 2010 Dietary Guidelines for Americans (DGAD), and a typical western diet (WD). In a three-period crossover trial, 55 subjects were randomly assigned to one of six possible sequential orders for eating each diet (KD, DGAD, and WD) for 4 weeks, separated by a 2-week rest. Samples were collected before and end of each diet period. Using ¹H NMR and 16S rRNA-targeted sequencing, metabolites and gut microbiota were profiled. Multivariate analysis showed discriminated metabolic pattern between before and after samples in every diet. Pathway analyses revealed that the most enriched metabolic pathway was valine, leucine and isoleucine biosynthesis in KD; synthesis and degradation of ketone bodies in DGAD and WD. Particularly, KD decreased plasma branched-chain amino acids (BCAA), such as leucine, isoleucine, and valine, which is related to obesity metabolism. Whereas DGAD and WD increased plasma ketone bodies, such as acetate, 3-hydroxybutyrate, 2-aminobutyrate, and acetone related to lipid metabolism. Also, in correlation analysis of metabolome and gut microbiota, plasma BCAAs were negatively correlated with *Bifidobacterium* only after KD intervention. Trimethylamine N-oxide, betaine, and choline were positively correlated with gut microbial lipid metabolism only after WD intervention. This study demonstrates that the analysis of the host metabolism and gut microbiota provide insight into the relationship between dietary patterns and risk of metabolic disease.

Poster Presentation : **ANAL.P-325**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optical Anisotropy of Core-Shell or Yolk-Shell Ag@Fe₃O₄ Nanochains

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Optical anisotropy of 1-dimensional nanochains of yolk-shell (YOSH) and core-shell (COSH) Ag@Fe₃O₄ nanoparticles (NPs) is attractive to comprehend electromagnetic relation in different materials in nanoscale regime. To investigate its unique properties, a YOSH Ag@Fe₃O₄ nanoscale superstructure is prepared through a successive process using COSH-NPs via a selective etching approach. The Ag-core can be etched when exposed to a mixture of polyvinylpyrrolidone (PVP) and hydrogen peroxide (H₂O₂) solution at 25 °C. It is investigated that the etching degree of Ag-core in the COSH-NPs is linearly correlated with the average molecular weight and amount of PVP and H₂O₂. In the optical investigation, one-dimensional YOSH and COSH nanochains are compared to show the dependence of anisotropic plasmonic response on tuning polarized light angle. The YOSH nanochain shows an insensitive plasmonic shift in respect of varying refractive index of solvent, which is probably related with the void of Ag-yolk and Fe₃O₄ shell. It is probable that the unique properties of the COSH and YOSH nanochain can be applied to be a potential photonic device and their ultralow quantity sensing and imaging.

Poster Presentation : **ANAL.P-326**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Magnetic nanozyme linked colorimetric assay for rapid diagnosis of infectious disease

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¹Chemistry, Chungnam National University, Korea

Development of a rapid and sensitive method for infectious disease diagnosis is highly important to prevent the further spread of disease and to enable effective clinical treatment. Herein, an ultrasensitive colorimetric approach combining the advantage of immunomagnetic nanobeads and the enzyme mimic activity of gold nanoparticles has been developed. Two kinds of amplification processes are used to enhance the detection sensitivity. The increased surface area and the magnetic properties enable the magnetic nanobead to catch a large number of antibodies and target viruses, thus very small amounts of the virus can be easily detected. And the signal amplification of nanozyme causing the enhancing of the optical signal. This approach could avoid complicate instruments and allowed detecting Influenza virus only by naked eyes as well as microplate reader. In addition, we introduced a novel practical approach to develop a robust sensing system, named magnetoplasmonic ELISA (magplas-ELISA), which collects and concentrates target antigen, and amplifies signal simultaneously. Gold nanoparticles (Au NPs) were decorated with the magnetic nanoparticles (MNPs) based on its ease of synthesis and bio-compatibility. It can replace peroxidase in colorimetric biosensor owing to its outstanding peroxidase-like activity. Our choice of MNP-Au NP has a triple function which is a capture probe, magnetic concentrator and signal amplifier in this system. Triple-functional- magnetoplasmonic NPs described here provides direct monitoring of biomarker in a clinical sample as urine and serum.

Poster Presentation : **ANAL.P-327**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Tuning plasmonic properties of 0-3D metastructure with self-assembled magnetoplasmonic nanoparticles

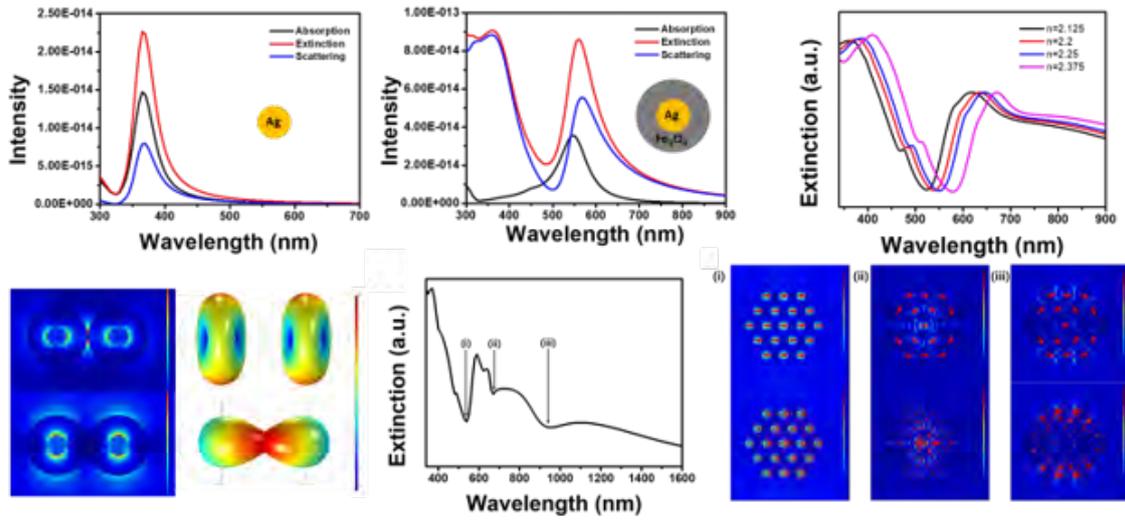
Dong-kyu Lee, Ki-Jae Jeong, Van Tan Tran¹, Jaebeom Lee^{2,*}

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Magneto-plasmonic nanostructures have been interested to the researchers in the fields such as optics, electronics and bio-engineering. They have been interested in its properties which can be explained with the concept of localized surface plasmon resonance. On the other side many researchers tried to fabricate metamaterials, the structure which shows abnormal optical property because of its permittivity and permeability which can be tuned by the periodic structures. We self-assembled nanoparticles into 1-3D suprastructure to make one kind of metamaterial. Moreover, we simulated absorption and scattering spectra of self-assembled suprastructure of Ag@Fe₃O₄ nanoparticles by using finite element method (FEM). We solved time-harmonic electromagnetic field distributions based on Maxwell's equation. We integrated energy loss on the surface and the volume of nanoparticles to plot extinction, scattering and absorption. Optical properties of single Ag@Fe₃O₄ nanoparticle in different condition was simulated. Moreover, 1-3D and chiral self-assembled structure of single nanoparticle was also simulated.



Poster Presentation : **ANAL.P-328**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optical analysis of degree of deacetylation in chitosan

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Chitosan is one of promising polymers for applications in various fields. However, despite diverse research studies conducted on its biocompatibility, its uses are still limited. The main factor that can affect its physical, chemical and biological properties is the degree of deacetylation (DOD), which represents the proportion of deacetylated units in the polymer. In this article, the in vivo biocompatibility of chitosan-hydroxyapatite composite films composed of chitosan with different DOD values was investigated by traditional biological protocols and novel optical spectroscopic analyses. The DOD of the chitosan was estimated and calculated by Raman spectroscopy, Fourier transform infrared spectroscopy, and proton nuclear magnetic resonance spectroscopy. The chitosan with the higher DOD induced a higher incidence of inflammation in skin cells. The amino group density, biodegradability, and crystallinity of chitosan are three possible factors that need to be considered when determining the biocompatibility of the films for in vivo application, since they led to complicated biological results, resulting in either better or worse inflammation even when using chitosan products with the same DOD. This basic study on the relationship between the DOD and inflammation is valuable for the development of further chitosan-based researches.

Poster Presentation : **ANAL.P-329**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of whitlockite nanoparticles in tri-solvent system as novel bone regenerative materials

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¹*Chemistry, Chungnam National University, Korea*

Whitlockite (WH, $\text{Ca}_{18}\text{Mg}_2(\text{HPO}_4)_2(\text{PO}_4)_{12}$) as the second most abundant biominerals in human bone has been attracted recently as an advanced bone graft material for regeneration and fillers in orthopedic and dental treatment. However, it still remains challenging to investigate the mechanism of crystal formation in pure phase WH nanocrystals and controlling its morphology as well as its biomedical applications. In this study, WH nanoparticles were synthesized in solid-liquid-solution (SLS) tri-solvent system. Precursor's ratio, interfaces between the surfactant and the WH crystals are optimized to grow WH nanocrystals with tunable sizes and morphology, and different surface properties. Computational finite element method (FEM) simulations were carried out to reveal the solvent effect in the reaction. Molecular dynamics (MD) simulations explained the growth mechanism of WH nanoplates (M1.5). Furthermore, the biological compatibility of the newly synthesized WH is evaluated in human osteosarcoma cell line (MG 63) treated with 100 $\mu\text{g}/\text{ml}$ up to 7 days. The cell proliferation and alkaline phosphatase (ALP) activity assay of human turbinata-derived mesenchymal stem cells (hTMSCs) demonstrated that WH can positively enhance the proliferation and osteogenic differentiation of stem cell. The as-synthesized WH through the new reproducible and robust route is biocompatible, cell-adhesive, and spreadable, which holds a promise to apply for further osteogenic tissue engineering.

Poster Presentation : **ANAL.P-330**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Electrochemical Immunosensor using Nanotriplex of Graphene Quantum Dots, Fe₃O₄, and Ag Nanoparticles for Tuberculosis

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Electrochemical technique is one of the powerful tools for characterization of NPs. The techniques have the potential to achieve rapid, sensitive, selective, and low-cost detection of biomolecules relevant to disease detection and diagnosis. Here, an electrochemical biosensor was developed for detection of mycobacterium tuberculosis (Mtb) antigen (CFP-10) using Fe₃O₄@Ag/GQD modified glassy carbon electrode (GCE) as a sensing platform and gold nanoparticles (AuNPs) as a label for signal amplification. The sensing platform was newly designed to obtain synergetic performance using three different nanomaterials; i.e., Fe₃O₄ for the purpose of increasing surface to volume ratio that strongly adsorb chemicals and rapidly transfer electrons, Ag for enhancing electrical conductivity to facilitate transfer of electrons and GQD increases surface area for capturing numerous primary antibodies (Ab1). A sandwich type immunoassay was prepared by immobilizing antibody 1 (Ab1), and AuNPs functionalized with antibody 2 (Ab2–AuNPs) on Fe₃O₄@Ag/GQD modified GCE. The immunosensor showed a wide linear range (0.005 - 500 µg/mL) with a limit of detection (LOD, S/N = 3) reaching 0.33 ng/mL. The result showed good performance with a high selectivity, and simple operation, can be easily extended to other pathogenic bacteria detection.

Poster Presentation : **ANAL.P-331**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication and Application of Microfluidic Devices to Test the Phototoxicity of Cosmetic Ingredients

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We describe the development and application of a compartmented microfluidic device for in vitro phototoxicity test. The microfluidic device consists of three compartments, with the outer compartments on both sides being cell culture channels and the middle compartment being the channel to regulate fluid flow. Human keratinocyte cells and human dermal fibroblast cells were cultured in the outer compartment of the microfluidic device. When all cells cultured in both compartments reached confluent state, a cell culture medium containing the test reagent was injected and irradiated with ultraviolet light (UVB) at 40 mJ/cm². In order to investigate the correlation between interleukin 8 (IL-8) secretion and phototoxicity, a human IL-8 ELISA kit was used to detect secreted IL-8 according to each experimental condition. In addition, the morphology of each cell cultured under the independent culture condition and the co-culture condition of two kinds of cells was observed. In the case of keratinocytes, proliferation and cluster formation were observed by stimulation of substance and UVB under independent culture condition, and more serious proliferation and cell death were observed in co-culture condition. In the case of dermal fibroblasts, cell necrosis was observed by stimulation of substance and UVB under independent culture condition, but in the co-culture condition, cells were observed to grow and proliferate similar to normal cells. The compartmented microfluidic device described in this study can be used as an alternative test method for evaluating the phototoxicity of cosmetics and cosmetic ingredients and can be used as an experimental device to observe intercellular interactions through co-culture of two kinds of cells.

Poster Presentation : **ANAL.P-332**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Stepwise Intact Protein Analysis for Quality Assessment of Therapeutic Glycoprotein with Complex Glycoform

Myung Jin Oh, Nari Seo, Hyun Joo An*

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

The glycosylation pattern of biotherapeutics is considered to be a very important attribute due to its strong effect on quality, stability, safety, immunogenicity, pharmacokinetics, and potency. In order to control of glycosylation as well as ensure the quality of drug, a systematic review for glycosylation on biotherapeutics from early stages of drug development to post-approval batch release is absolutely required. Here, we have developed stepwise strategies for glycome quality assessment during drug design and manufacturing in the level of intact protein. The first step, on-line desalting, and diphenyl based nano-LC/Q-TOF MS were employed for the determination of molecular weight with various glycoforms, glycosylation site occupancy, and carbohydrate contents. The second step, overall O-glycoform and non-glycosylated protein portion were examined by N-deglycosylated protein analysis. In addition, bottom-up data was used to refine information gained at the intact protein level. The global glycosylation profile for each production batch was obtained by intact protein analysis, and comparisons of the glycoform profiles from different lots were made based on the deconvoluted intact mass spectra. This approach could be widely applied for real-time monitoring and direct comparison of glycosylation throughout the drug pipeline.

Poster Presentation : **ANAL.P-333**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development anti-oxidant chemical compound from natural product and identification of its mechanism

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

This research aims to screen biocompatible antioxidant chemical compounds that can be used for cosmetic raw resource as an anti-aging functional material. Basically ninety-six whole extract samples were supplied from Korea National Institute of Biological Resources and extract were obtained all from plant resources that collected from southeast Asian countries including Vietnam, Cambodia, Thailand and Myanmar. Collected-raw materials were extracted in 70% ethanol extract and concentrated samples were validated to identify anti-oxidant activity using conventional ABTS [2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)] assay. Then, twenty-two samples were shown excellent antioxidant activity and they were characterized in human keratinocyte (HaCaT cells) to investigate inhibitory activity against reactive oxygen species (ROS) formation by UV-irradiation. After ABTS assay, sample No.4 have shown strongest antioxidant effect in HaCaT cells and whole extract was fractionated using HPLC with C18 column. Then active fraction was characterized to identify their chemical structure using NMR and mass spectrophotometry.

Poster Presentation : **ANAL.P-334**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Absolute Quantitation of Non-Human Glycan (Neu5Gc) in Human Biopsy Tissue by LC/MRM-MS

Nari Seo, Myung Jin Oh, Hyun Joo An*

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N-Glycolylneuraminic acid (Neu5Gc), which cannot be synthesized in human, is an immunogenic sugar of dietary source. Neu5Gc in blood and tissue metabolically promote a variety of cell-to-cell adhesion processes in inflammation and the immune response related to cancer, cardiovascular, and inflammatory diseases. Thus, Neu5Gc in human has been considered as the indication of inflammation-mediated diseases, and their level has attracted more attention for monitoring disease progression and/or response to therapy. Although several Neu5Gc quantitation methods have been proposed for disease marker, determination of the levels of Neu5Gc in individual human samples is still challenging because there are very low amounts of Neu5Gc (less than 0.01% of the total sialic acids). Here, we have developed the MRM-based assay for the first time to quantify Neu5Gc from one shot biopsy gastric tissues, proved that the amount of Neu5Gc was correlated with cancer. Gastric biopsy tissues of cancer patient (n=10) and healthy control (n=10) were obtained from Seoul National University Bundang Hospital in Korea. Each tissue (2-3 mg wet wt.) was chemically treated. Liberated Neu5Ac and Neu5Gc were chromatographically separated, then monitored by LC/MRM-MS. The quantitative calibration curve of Neu5Gc was linear over the range of 1.5 fmol/L to 1.5 $\mu\text{mol/L}$ (10^3) and its correlation coefficient (r^2) was >0.999 . Neu5Gc was successfully quantified in all samples from gastric cancer patients and healthy controls, and the concentration of Neu5Gc was determined at fmol levels per one biopsy tissue. When compared to absolute abundances of Neu5Gc between controls and patients, expression levels in patient cohorts were 1.5 to 2-folds higher than those in the control group. These results could be supporting that the existence of Neu5Gc in human is linked to the disease. The developed strategies might be a new paradigm for a complement to glyco-based current cancer screening platform.

Poster Presentation : **ANAL.P-335**

Analytical Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Ultrasound-controlled chiral separation of four amino acids and 2,2,2-trifluoro-1-(9-anthryl)ethanol

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

In order to efficiently separate various chiral samples, it is highly important to select appropriate mobile phase and stationary phase suitable for each analyte. Many efforts have been made to improve separation factor and reduce analysis time on liquid chromatography. Ultrasound is widely used in the fields of medicine, pharmacology, cosmetics, food and various industries. Many studies have been conducted by using ultrasound with chromatography to date so as to improve the extraction efficiency in the sample preprocessing stage. Since Okada first attempted to investigate the influence of ultrasound in ion-exchange chromatography, our research team has conducted several studies for chiral separation using ultrasound. In the previous studies, we found that ultrasound decreased retention time in chiral chromatography at several temperatures and improved enantioselectivity at high temperatures. In this study, we investigated the influence of temperature (25 °C, 50 °C) and ultrasonication (25 kHz) on chromatographic separation for α -amino acids on ChiroSil®RCA(+) and 2,2,2-trifluoroanthrylethanol (TFAE) on C3 symmetric CSP4 columns. In addition, separation factor and resolution was observed according to different watt density conditions at both temperatures and ultrasound-controlled method was applied as new one for better selectivity and resolution.

Poster Presentation : **LIFE.P-336**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

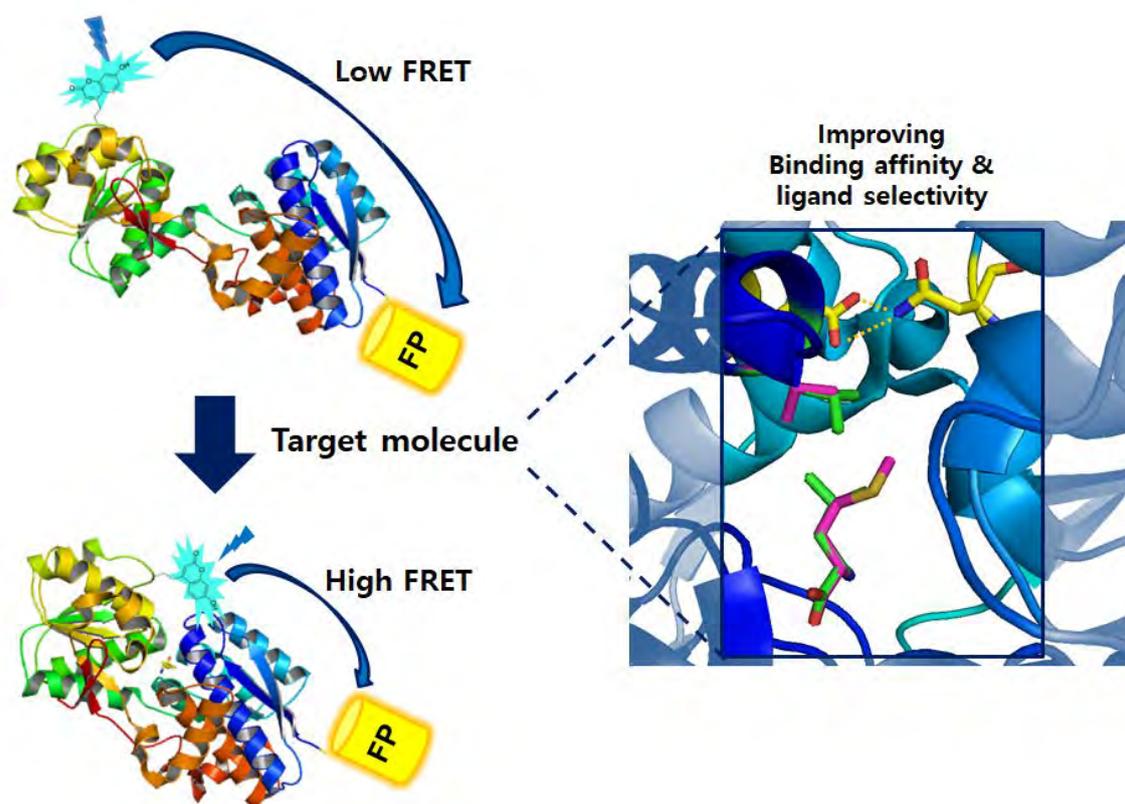
Engineering a periplasmic binding protein for amino acid sensors with improved binding properties

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Periplasmic binding proteins (PBPs) are members of a widely distributed protein superfamily found in bacteria and archaea, and involved in cellular uptake of solute. In this study, glutamine binding PBP (GlnBP) and leucine binding PBP (LeuBP) were engineered to detect L-Glu and L-Leu by FRET change upon ligand binding. A fluorescent unnatural amino acid, L-(7-hydroxycoumarin-4-yl)ethylglycine (CouA), was genetically incorporated into the protein as a FRET donor, and emerald green fluorescent protein (EGFP) or yellow fluorescent protein (YFP) was fused to its N-terminus as a FRET acceptor. The best sensor protein showed 1.5-fold increase in FRET ratio. In the case of leucine sensor protein, its substrate specificity was significantly improved by engineering the LeuBP, showing minimal FRET ratio change with the other 19 natural amino acids and D-Leu. Further engineering made the sensor protein more sensitive (14-fold) for L-Leu, and recognize L-Met as well with moderate binding affinity. Selected mutant sensors were used to measure L-Glu and L-Leu concentration in a biological sample (fetal bovine serum) and optical purity of Leu and Met. This FRET-based sensor design strategy allowed us to readily engineer the natural receptor to have improved binding affinity and specificity, and to recognize other natural molecules which are not a ligand for the wild-type receptor. The design strategy can be applied to other natural receptors and would make it possible to engineer the receptors to sense biochemically more interesting molecules.



Poster Presentation : **LIFE.P-337**

Life Chemistry

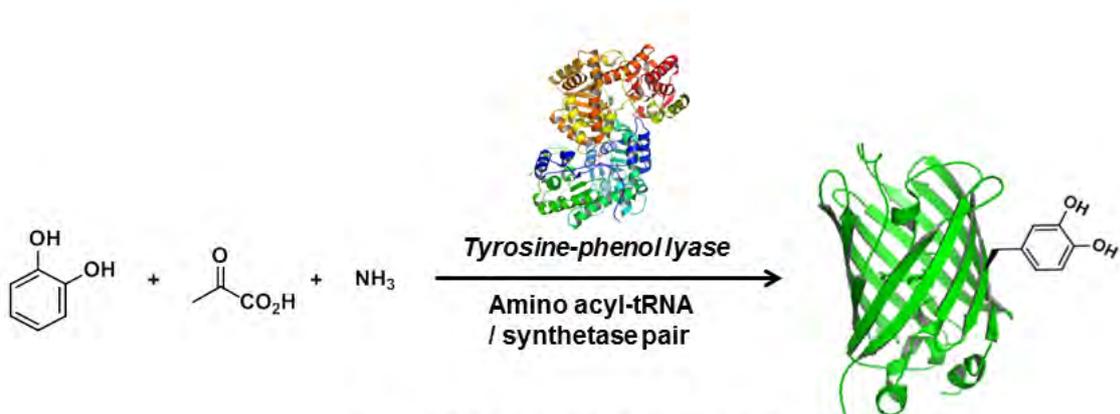
Exhibition Hall 2, FRI 11:00~12:30

Genetic Incorporation of Biosynthesized L-dihydroxyphenylalanine (DOPA) and Its Application to Protein Conjugation

Sang kil Kim, Hyunsoo Lee*

Department of Chemistry, Sogang University, Korea

L-dihydroxyphenylalanine (DOPA) is an amino acid found in the biosynthesis of catecholamines in animals and plants. Because of its particular biochemical properties, the amino acid has multiple uses in biochemical applications. This report describes a protocol for the genetic incorporation of biosynthesized DOPA and its application to protein conjugation. DOPA is biosynthesized by a tyrosine phenol-lyase (TPL) from catechol, pyruvate, and ammonia, and the amino acid is directly incorporated into proteins by the genetic incorporation method using an evolved aminoacyl-tRNA and aminoacyl-tRNA synthetase pair. This direct incorporation system efficiently incorporates DOPA with little incorporation of other natural amino acids and with better protein yield than the previous genetic incorporation system for DOPA. Protein conjugation with DOPA-containing proteins is efficient and site-specific and shows its usefulness for various applications. This protocol provides protein scientists with detailed procedures for the efficient biosynthesis of mutant proteins containing DOPA at desired sites and their conjugation for industrial and pharmaceutical applications.



Enzymatic reaction and genetic incorporation



Poster Presentation : **LIFE.P-338**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

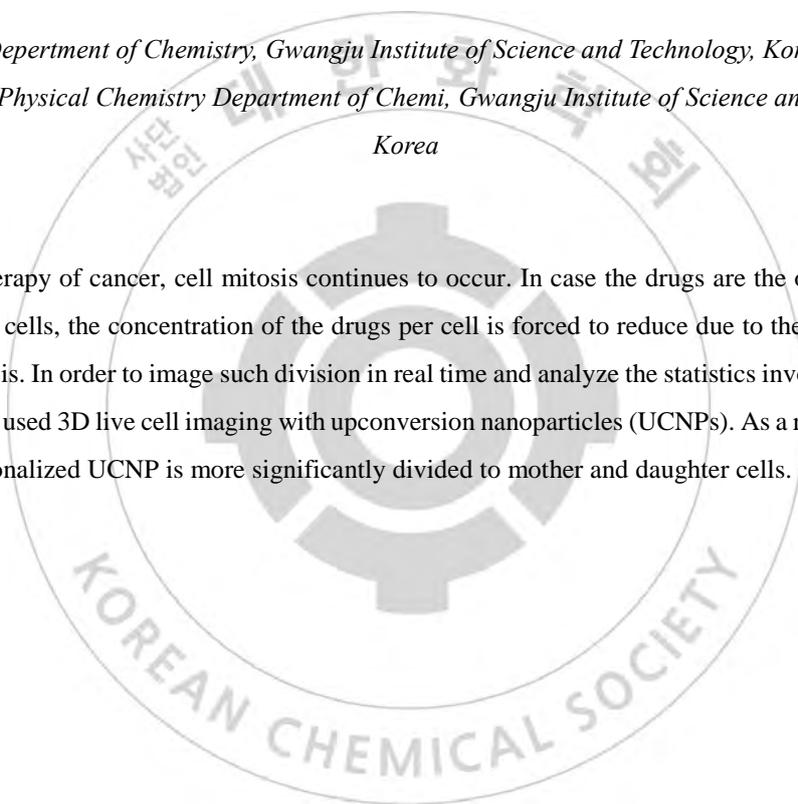
3D imaging of cancer cell mitosis with upconversion nanoparticles

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In chemical therapy of cancer, cell mitosis continues to occur. In case the drugs are the ones that require uptake into the cells, the concentration of the drugs per cell is forced to reduce due to the subsequent and continual mitosis. In order to image such division in real time and analyze the statistics involved in the drug partitioning we used 3D live cell imaging with upconversion nanoparticles (UCNPs). As a result, negatively charged functionalized UCNP is more significantly divided to mother and daughter cells.



Poster Presentation : **LIFE.P-340**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characterizing Hetero-oligomer from 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 ($A\beta$)" and "Alpha-synuclein (α -syn)", respectively which are believed to be primarily responsible for the pathogenesis. Further study showed that there are a large number of patients with symptoms of both diseases at the same time and these patients are known to have a faster disease progression and worse prognosis than pure AD or PD patients. It is also known that the rate of the oligomerization (or aggregation) increases when $A\beta$ and α -syn co-exist, and the co-existence causes the diseases to be even worse. It is very likely that hetero-oligomers could be formed, but the 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 the N-terminal of $A\beta$ and N-terminal of α -syn were conjugated at AFM probes, and the specific interaction between the antibodies and surface of the oligomers was observed^{1,2}. After adsorbing the oligomers on a mica surface, a tip tethering $A\beta$ 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 the two different antibodies were observed within an oligomer, and it holds true 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 recognized pixels for α -syn is higher than with the α -syn homo-oligomer, suggesting a different mode of aggregation for the hetero-oligomerization. We believe that such structural information will help to understand the relationship between the misfolded hetero-proteins and the pathogenesis in brain. References 1. Y. J. Jung, B. J. Hong, W. Zhang, S. J. Tendler, P. M. Williams, S. Allen, J. W. Park, *J. Am. Chem. Soc.* 129, 9349 (2007). 2. D. H. Kim, J.-E. Lee, Z.Y. Xu, K. R. Geem, Y. Kwon, J. W. Park, I. Hwang, *Nat. Commun.* 6,

6843 (2015). Acknowledgement This work is supported by the KGPF (Korea Global Ph.D. Fellows) from NRF (National Research Foundation of Korea).



Poster Presentation : **LIFE.P-341**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Quantification of Tumor-associated Circulating Free DNA with Atomic Force Microscopy

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Unlike conventional invasive biopsy method, non-invasive liquid biopsy has come into the spotlight to obtain information about cancer from present biomarkers such as circulating free DNA (cfDNA), exosomes, circulating tumor cells (CTCs) in patient's blood. Especially various methods that detect genetic alterations of circulating free DNA (cfDNA) can be used for diagnosis and prognosis of cancer. There have been many endeavors to reveal correlation between cfDNA and cancer in the past few years. Here we propose a new methodology using atomic force microscopy (AFM) to quantify tumor-specific genetic aberration involved in methylation change of cfDNA with very low abundance. Quantification of methylated cfDNA is under way by using MBD2 (methyl-CpG-binding domain protein2) having the ability to recognize symmetrically methylated single CpG and UHRF1 that recognizes hemimethylated CpG sites. This unprecedented liquid biopsy followed by AFM will be a great help for conquering cancer. Reference 1. Crowley, E.; Di Nicolantonio, F.; Loupakis, F.; Bardelli, A., Liquid biopsy: monitoring cancer-genetics in the blood. *Nat. Rev. Clin. Oncol.* 2013, 10 (8), 472. 2. Lee, Y.; Kim, Y.; Lee, D.; Roy, D.; Park, J. W., Quantification of Fewer than Ten Copies of a DNA Biomarker without Amplification or Labeling. *J. Am. Chem. Soc.* 2016, 138 (22), 7075-7081.

Poster Presentation : **LIFE.P-342**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Quantitative Analysis of LIMK1 in a Single Cell with Atomic Force Microscopy

Ji-seon Lim, Joon Won Park*

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Proteins are essential parts of organisms and participate in virtually every process within cells, performing a variety of functions. LIMK1 is a multifunctional protein and is involved in regulation of cell motility, cell cycle, cytokinesis and cellular morphology. LIMK1 also regulates neurite growth, synaptic stability, growth cone motility, axon formation through modulation of Golgi dynamics and neuronal differentiation. This protein stimulates axon growth and may play a role in brain development. In particular, LIMK1 hemizyosity is implicated in the impaired visuospatial constructive cognition of Williams syndrome, which is a unique neurodevelopmental disorder characterized by severe defects in visuospatial cognition and long-term memory. Accordingly, quantitative analysis of LIMK1 and their distribution in a single cell is important to study the biological role of LIMK1 in neurons. Conventional methods for protein analysis including western blotting, ELISA, and immunofluorescence have some problems that they have low detection limit and use fluorescent molecules. Therefore, atomic force microscopy (AFM) is a good candidate to overcome the hurdles. Using the mapping capability of AFM, it is possible to obtain a map the distribution of a specific protein in a nanometric resolution without modification or amplification. In this way, LIMK1 can be analyzed quantitatively in a single cell and their distribution can be mapped at high lateral resolution.

Poster Presentation : **LIFE.P-343**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Methodology Development of Screening Weak Binders by Using NMR Spectroscopy

Yoonjin Um, Young Kee Chae*

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We have been developing a novel screening approach by using NMR spectroscopy. Our method is based on the hypothesis that any molecule that binds to a very large target protein will lose its NMR signal due to a very slow tumbling rate, which is a fundamental phenomenon of NMR spectroscopy. Our goal is to screen as many molecules as possible in a super high throughput fashion. After finding weak binders, the next move will be to combine those molecules to make stronger binders that can then be applied pharmaceutically. Our approach to make a very large target protein is through the formation of the supramolecular complex by using a polypeptide (ELP) that tends to aggregate, not get denatured, at slightly elevated temperatures. To prove our hypothesis, we chose 2 proteins as testable targets: the maltose binding protein (MBP) and glutathione S-transferase (GST). We fused those two proteins to an ELP. To prepare a ligand pool that can be screened by using a simple NMR technique, we labeled the candidate molecules with C-13 by feeding E. coli or yeast with C-13 glucose as a sole carbon source. Our preliminary data shows that MBP picked up one compound whose signal disappeared as we expected, and we are now in the process of identifying it. We hope this new approach will provide an alternative way to design suitable compounds from a pool of weak binders. 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).

Poster Presentation : **LIFE.P-344**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Construction of Auto-Inducible Promoters for Recombinant Protein Production

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The production of recombinant proteins in *E. coli* involves such factors as host strains, expression vectors, culture media, and induction methods. The typical approach to producing heterologous proteins consists of the followings: (1) insertion of the target gene into a suitable vector, (2) transformation of a strain specialized for protein production with the resulting plasmid DNA, (3) growth of the host in a suitable medium and induction of the protein production at a right moment, and (4) further growth to get the maximum yield. We constructed expression plasmids with auto-inducible promoters working in a host that is not specialized for protein production, and in a TB medium which does not contain any secret ingredient. This plasmid also contains the color indicator which turns red when protein production is successful. We hope that these plasmids will help academic and industrial researchers save their time and effort in a routine protein production procedure. 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).

Poster Presentation : **LIFE.P-345**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mimicry of the Cytoskeleton; Actin-microtubule co-formation in a Giant Unilamellar Vesicle

Sungwoo Jeong, ChangHo Kim¹, Huong Thanh Nguyen², Agustina Setiawati¹, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

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²*Chemistry, Sogang University, Korea*

Microtubule and actin cytoskeletons are physically contacted in a cell and dynamically coordinated to play vital roles in many cell functions, from migration, growth, and division. These structural dynamics of cytoskeletal proteins are of interest, the physical roles of cross-linking proteins between two filaments have been identified. Yet most studies were performed in a highly controlled interface or a bulk. Recently, we developed to simulate a cytoskeleton formation through ATP-dependent actin polymerization in a giant unilamellar vesicle. Optical stimulation initiated ATP synthesis and induced ATP-dependent actin polymerization, leading to the growth of three-dimensional highly curled actin filament network. In this study, we further added the ingredients for microtubule formation into the actin polymerizable GUV system and initiated the filament formation of those two cytoskeleton proteins simultaneously. We will discuss how these highly curled actin filaments in the single vesicle affect the structural environment in the presence of highly straight microtubule filaments. We will discuss how these two filaments are interacting in a highly confined, cell-like space where they are mutually restricted in further research.

Poster Presentation : **LIFE.P-346**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Co-formation of actins and microtubules; interaction and morphological aspects.

ChangHo Kim, Sungwoo Jeong¹, Kwanwoo Shin^{1,*}

Institute of Biological Interfaces, Sogang University, Korea

¹Department of Chemistry, Sogang University, Korea

The cytoskeleton in cell consists of three filamentous subsystems, microtubules, actin filaments and intermediate filaments. These have been studied for decades in cell, microtubule and actin in cytoskeleton play an important role in cell migration, division and cell shape changes. Microtubule and actin filament crosslink with coupling proteins or physically contact to perform an important role in cell functions. These coupling proteins for crosslink and mechanisms of actin-microtubule crosslinking have been studied and identified, but these studies were not performed in a highly controlled interface or a bulk. So, we developed to simulate a cytoskeleton formation through ATP-dependent actin polymerization and GTP-dependent microtubule polymerization in a bulk and a giant unilamellar vesicle. This research is restricted within the results in a bulk. For the results of a giant unilamellar vesicle, you can see on other poster of co-member. We represent actin polymerization, microtubule polymerization controlled with ion (Mg^{2+} , Ca^{2+}) concentration and actin-microtubule polymerization in a bulk. We will discuss the interaction and mechanism of actin-microtubule crosslinking in a bulk and in a highly confined as cell through a giant unilamellar vesicle on next time.

Poster Presentation : **LIFE.P-347**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Antidiabetic effect of CBL through inhibition of protein tyrosine phosphatases relevant to insulin resistance

Sang Jeon Chung*, **Ji Young Hwang¹**, **Do Hee Ahn²**, **Se Jeong Kwon³**

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²*Pharmacy, Sungkyunkwan University, Korea*

³*pharmacy, Sungkyunkwan University, Korea*

We have identified PTPN9 and DUSP9 as potential antidiabetic targets. In this study, PTPN11 knockdown increased AMPK phosphorylation, indicating that PTPN11 could be an antidiabetic target. A library of 658 natural products was screened to identify the inhibitors of PTPN9, DUSP9, or PTPN11. Among the PTP-inhibitory compounds, CBL showed a strong inhibitory activity against PTPN9 and PTPN11, meaning that it would be a potential antidiabetic candidate with a dual targeting of those PTPs. The inhibitory activities of CBL against PTPN9 and PTPN11 were determined to be $K_i = 3.4$ nM and $K_i = 67.4$ nM, respectively. Furthermore, CBL stimulated glucose uptake and resulted in increased AMP-activated protein kinase (AMPK) phosphorylation. Taken together, we demonstrated that CBL, as an inhibitor of PTPN9 and PTPN11, increased glucose uptake through activation of the AMPK signaling pathway. These results strongly suggest that CBL could be used as a potential therapeutic candidate for the treatment of type 2 diabetes.

Poster Presentation : **LIFE.P-348**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Screening and characterization of MAP kinase-interacting kinase 1(MNK1) using homogeneous time-resolved fluorescence resonance energy transfer (TR-FRET)

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Department of Chemistry, Keimyung University, Korea

MAP kinase-interacting kinase 1 (MNK1) is a serine/threonine-protein kinase that regulates protein synthesis by phosphorylating eukaryotic translation initiation factor 4E (eIF4E). Overexpression of eIF4E has been reported to play a major role in the development of various cancers such as breast, colon, prostate, head and neck, kidney and lung. Therefore, MNK1 has drawn attention as an important target for cancer treatment. Using the TR-FRET assay method, we performed screening of a kinase focused library 333 compounds at 10 μ M concentration and found a series compounds that effectively inhibited the activity MNK1. It was found that 4-substituted-2-amino pyrimidine structures were common cores in these hits. The Lineweaver-Burk double-reciprocal plot and Nonlinear regression analysis of KMU010348, the most potent inhibitor of MNK1 inhibition, revealed that this compound is a competitive inhibitor of ATP.

Poster Presentation : **LIFE.P-349**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Identification and Characterization of Novel Leads from a Kinase-Focused Compound Library for Hepatocyte Growth Factor Receptor (HGFR)

Hyun Ho Jeong, Jinho Lee*, Victor Sukbong Hong*

Department of Chemistry, Keimyung University, Korea

Hepatocyte growth factor receptor (HGFR), also called c-MET, is a transmembrane tyrosine kinase which is encoded by the *MET* gene. HGFR is associated with cell proliferation, motility, migration and invasion. Although HGFR plays an important role in regulating tissue homeostasis, it is also known that overexpressed HGFR has been implicated in cancer angiogenesis and metastasis. Hence, development of small molecular inhibitors to block the activity of HGFR can be a good way to treat the cancer. We have used a time-resolved fluorescence resonance energy transfer (TR-FRET) assay to identify small molecule inhibitors of HGFR. By screening a kinase-focused library of 333 compounds at 10^{-6} M concentration, we identified a group of compounds with a 3,4,5-trisubstituted indoline as a common core structure that inhibits HGFR activity. To understand the mechanism of inhibition of 3,4,5-trisubstituted indoline against HGFR, we carried out mechanistic studies with KMU010642 which is the most potent compound from screening. Kinetic analysis demonstrates that KMU010642 is competitive with ATP.

Poster Presentation : **LIFE.P-350**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Modulation of Cell Alignment Using Patterned Surface Charge without Topographical Depth Difference

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Biomedical Research Institute, Korea Institute of Science and Technology, Korea

¹Department of Chemistry, Hanyang University, Korea

Modulating the morphology of surface has been widely employed as a versatile tool for spatially controlling cell's growth, adhesion, and alignment based on the understanding of the interaction between cells and surface. Among many morphological modification, the strategy using various microgroove patterns has been widely applied. However, this strategy using various microgroove patterns is challenging to provide the environment for intercellular communications to maintain homeostasis due to the difference of depth between patterns. Herein, we report the alternative surface modification methods able to spatially control cell alignment and provide the environment for cell-cell communications as well, avoiding geometrical variations. The various patterns of the surface that consist of periodic areas with different charges were fabricated using photolithography and nanoparticle with charged ligands. The cells on the charged pattern without topographical depth difference showed aligned with orientation along the lines of the pattern. The surface can provide the more improved environment to communicate with gap junctions than the groove patterns surface. This strategy using the difference of charge density pave a new way to control the cell behavior on surfaces, providing the environment for intercellular communications.

Poster Presentation : **LIFE.P-351**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Identification of KDHO1 via inhibition of the protein tyrosine phosphatase VHR as an anti-tumor drug

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¹*College of Pharmacy, SungKyunKwan University, Korea*

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 associated with many human diseases including cancers, diabetes, and inflammatory disorders. Dual specificity protein phosphatase 3 (DUSP3, also named VHR; Vaccinia-H1 related) has been shown to negatively regulate members of the mitogen-activated protein (MAP) kinase superfamily (MAPK/ERK, SAPK/JNK, p38) involved in cellular proliferation and differentiation. VHR is known to be highly expressed in several cervix cancer cell lines such as HeLa. In this study, KDHO1 isolated from *Paeonia lactiflora* was identified as the inhibitor for VHR with subnanomolar K_i value. In addition, we used a cell culture system treated with KDHO1 to demonstrate its specificity and possibility for anticancer drug. These results identify potential new therapeutic strategies for cancer treatment.

Poster Presentation : **LIFE.P-352**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Antibacterial nanoparticles: enhanced antibacterial efficiency of coral-like crystalline rhodium nanoplates

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¹*Department of Applied Chemistry, Kyung Hee University, Korea*

This paper deals with the newly found antibacterial efficiency of coral-like crystalline Rh nanoplates. Results clearly demonstrate that the composition and morphology of a nanostructure play significant roles in antibacterial effects.



Poster Presentation : **LIFE.P-353**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Thermochromic indicator for determination of optimal fruit taste

Yong-Hoon Kim*, **June Hyuck Park**

National Institute of Agricultural Sciences, Korea

Thermochromic indicator exerting temperature-dependent color switching behavior has been applied to various industrial fields due to the easy detection, safety, and low cost. In line with consumer demands for healthier, safe, and high quality products, smart food-packaging technology has been developing such as fresh and ripeness indicators. Here, we introduce the naked-eye discernible indicator for informing the optimal intake temperature of a fruit. This attachable indicator is fabricated by a commercialized printing method which is able to adjust the visibility through applied ink thickness. At the thickness of 20 – 25 μm , the temperature-dependent visibility is favorable. When a chilled fruit is naturally heated under the room temperature, the indicator attached on the surface of fruits shows the three-color switching behaviors, violet, red, and gray, in variation with temperature. The indicator displays the red color at the optimal fruit temperature for intake. The temperature difference between the sensor and the surface of fruit is below 1 $^{\circ}\text{C}$. Heat transfer process between atmosphere and fruit is investigated on the basis of Newton's cooling law.

Poster Presentation : **LIFE.P-354**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

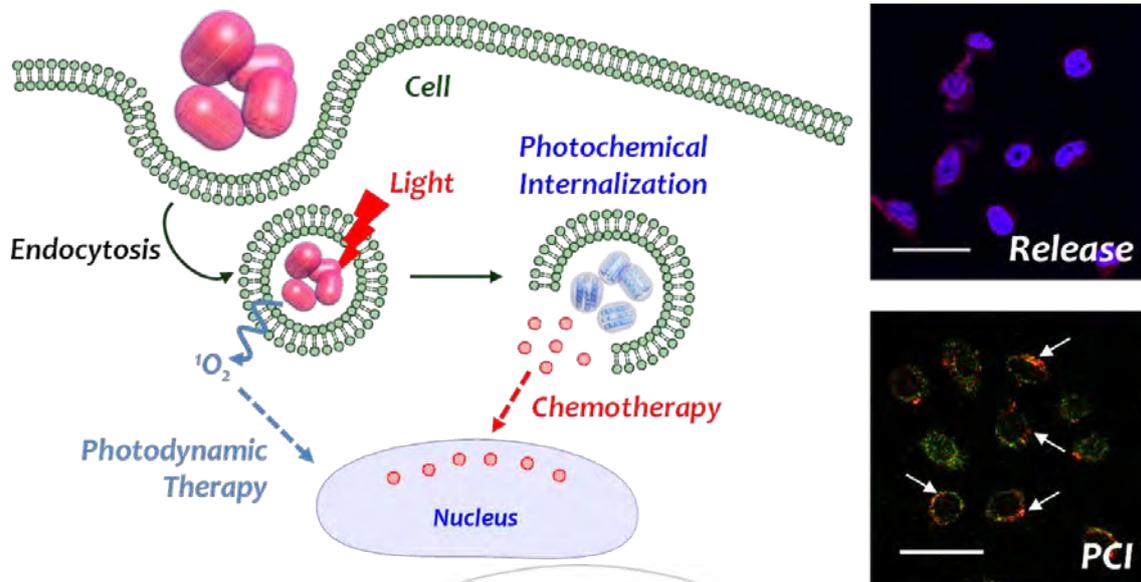
Photodynamically assisted chemotherapy by drug/photosensitizer co-loaded silica nanoparticle coated with $^1\text{O}_2$ -labile polymer

Junseok Lee, Won jong Kim^{1,*}

Pohang University of Science and Technology, Korea

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

Although chemotherapy is strong enough by itself to be a major of anti-cancer therapy, recent approach has been focusing on grafting various techniques such as nanotechnology to enhance the therapeutic effect and reduce the side effect. For instance, a controlled release of drug, an enhanced circulation, or an addition of additional therapeutic methods including photothermal and photodynamic therapy can be easily rendered by nanoparticle-based chemotherapy. Herein we report photodynamically assisted chemotherapeutics fabricated by drug and photosensitizer co-loaded nanoparticle coated with a stimuli-responsive polymer shell. A typical photosensitizer chlorin e6 (Ce6) was conjugated on the vertical channel of mesoporous silica and an anticancer drug doxorubicin was co-loaded in the pore. The nanoparticle (CeAP-L-PEG) was covered by polyethylene glycol (PEG) conjugated with singlet oxygen cleavable linker, bis(alkylthio)alkene. Upon irradiation of the red light (660 nm), generation of singlet oxygen greatly facilitated both release of the drug triggered by deshielding of the polymer shell followed by endosomal escape of the drug, which was leading to enhanced anticancer effect observed in vitro and in vivo. Taken together, our rationally designed nano-reservoir system signifies therapeutic potential of nanoparticle-based photodynamic therapy for effective cancer chemotherapy.



Poster Presentation : **LIFE.P-355**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Self-degradable Graphene Nanomedicine Operated by DNAzyme for Cancer Therapy and Clearance

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¹*Pohang University of Science and Technology, Korea*

It has drawn great interest in drug delivery to fabricate multifunctional nanomedicine for cancer therapy. Graphene oxide (GO) have attracted much attention in biomedical applications due to mechanical and chemical stability, abundant oxygen functional groups on large surface area, and photothermal effect. However, recent studies have shown that GO accumulates in certain organs, which can cause potential toxicity. G-quadruplex (G4)/hemin-based DNAzymes have been known for their peroxidase activity mimicking the horseradish peroxidase (HRP). Herein, we designed GO-G4-hemin complex for enhanced anticancer therapy and clearance of nanomedicine. This conjugated duplex G4 sequence is employed for intercalation of anticancer drug between DNA base pair, enabling anticancer drug release and formation of G4/hemin complex upon irradiation with infrared light. The G4/hemin complex bound to GO induced the oxidation and degradation of GO in hydrogen peroxide-rich tumor microenvironment. The described nanomedicine provides a versatile platform for stimuli-responsive cancer therapy and clearance.

Poster Presentation : **LIFE.P-356**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

pPBA@TiO₂-doxorubicin nanoparticles for targeted chemodynamic therapy of cancer

Seonil Kim, Sooseok Im¹, Junseok Lee¹, Won jong Kim*

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Ultrasound can penetrate much deeper in biological tissue because it is non-radiative and has a low tissue attenuation coefficient. The ability of ultrasound to activate some sensitizer such as porphyrin, titanium dioxide nanoparticle has led researchers to consider sonodynamic therapy (SDT) as a possible alternative to photodynamic therapy. Herein, we designed a ROS stimuli-responsive self-assembled nanoparticle that can be activated by ultrasound to generate ROS. Doxorubicin(DOX), a kind of anticancer drug, loaded titanium dioxide nanoparticle(TNP) are wrapped by polymerized phenyl boronic acid(pPBA). pPBA can interact with DOX by making phenyl boronic ester coupling, and this coupling is sensitive to ROS generated by TNP under ultrasound stimuli. Also, phenyl boronic acid can target cancer cell, containing many sialyated protein that interact well with PBA. This system has potential of tumor targeting drug delivery system that treat tumor by combination of SDT and chemotherapy.

Poster Presentation : **LIFE.P-357**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

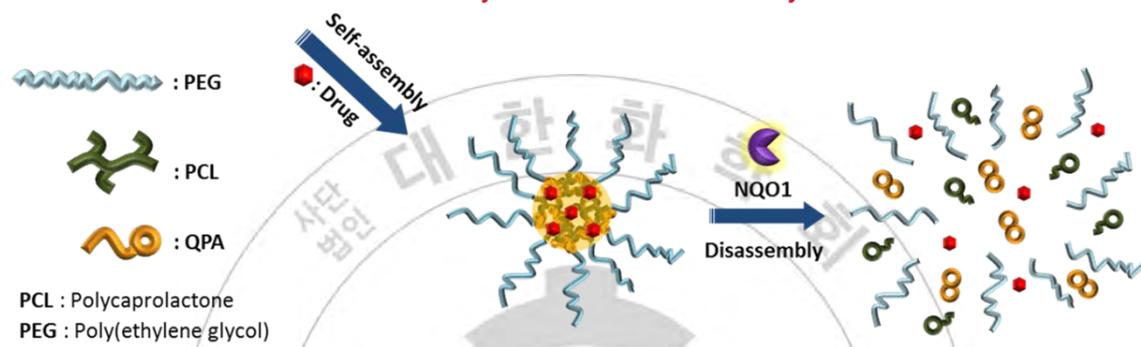
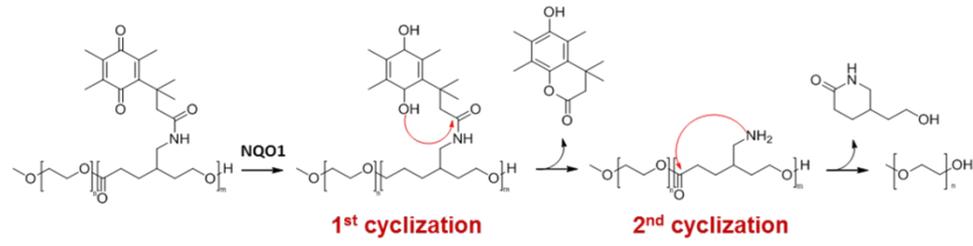
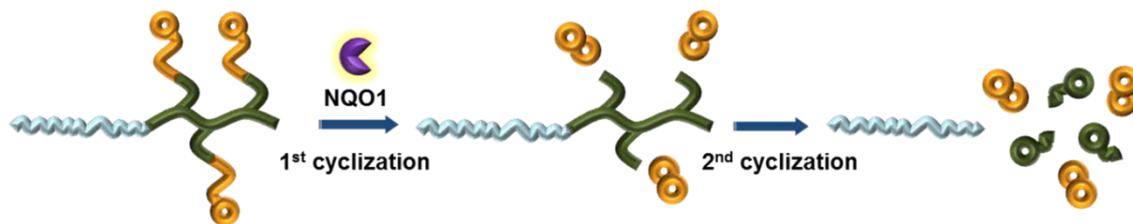
Enzyme-responsive Polymeric Micelles by Controlled Depolymerization for Anti-cancer Drug Delivery

Jaehyun Park, Won jong Kim^{1,*}

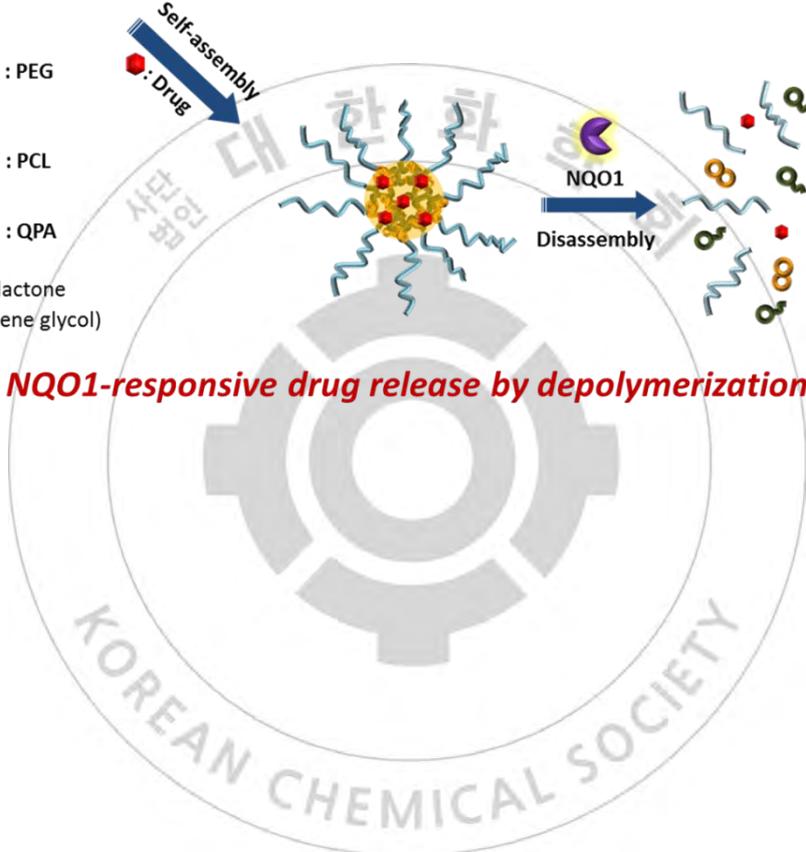
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The activity of high concentration of a specific enzyme in cancer has been utilized in a diagnosis of cancer, as well as cancer-targeted drug delivery system. NAD(P)H:quinone oxidoreductase-1 (NQO1), an over-expressed enzyme in certain cancer cells, maintains homeostasis and inhibits oxidative stress caused by elevated reactive oxygen species in cancer cells. The activity of NQO1 in lung and liver cancer cells is increased up to 50 times than that in normal cells. Interestingly, NQO1 reacts with trimethyl-locked quinone propionic acid (QPA) and produce lactone-based moiety via intramolecular cyclization. Herein, we present a novel enzyme-responsive polymeric micelle which can undergo depolymerization in response to NQO1. The enzyme-responsive polymer (PEG-*b*-PCL-QPA) was successfully synthesized by ring-opening polymerization of QPA-amide protected polycaprolactone (PCL) using polyethylene glycol (PEG) as a macroinitiator. These amphiphilic block copolymers self-assemble in aqueous condition into micelles that can disassemble and release encapsulated drugs through depolymerization of the polymers upon activation of NQO1. Compared to control groups, enzyme-responsive micelle showed efficient drug release and enhanced anti-cancer effects in vitro. These results indicate that the enzyme-responsive polymeric micelles present a promising potential for improving the efficacy of anti-cancer drug delivery system.



NQO1-responsive drug release by depolymerization



Poster Presentation : **LIFE.P-358**

Life Chemistry

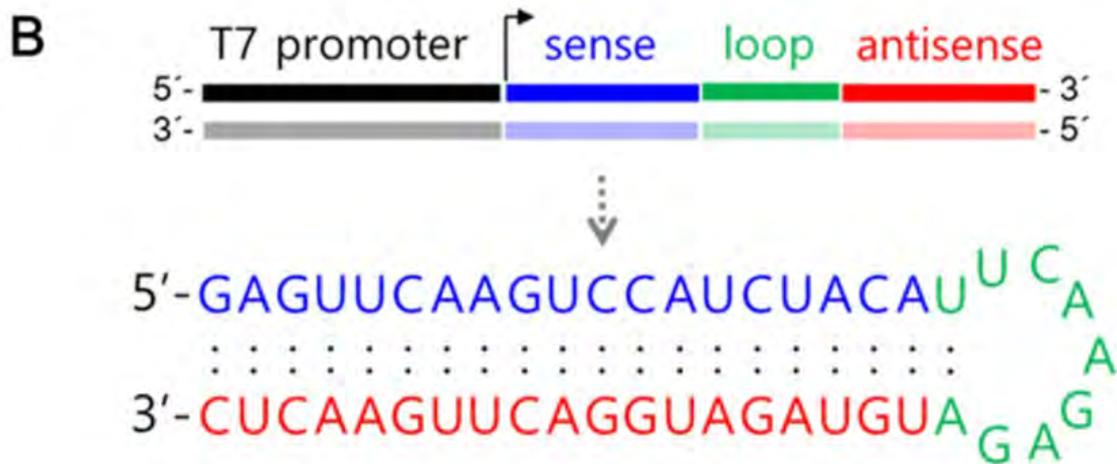
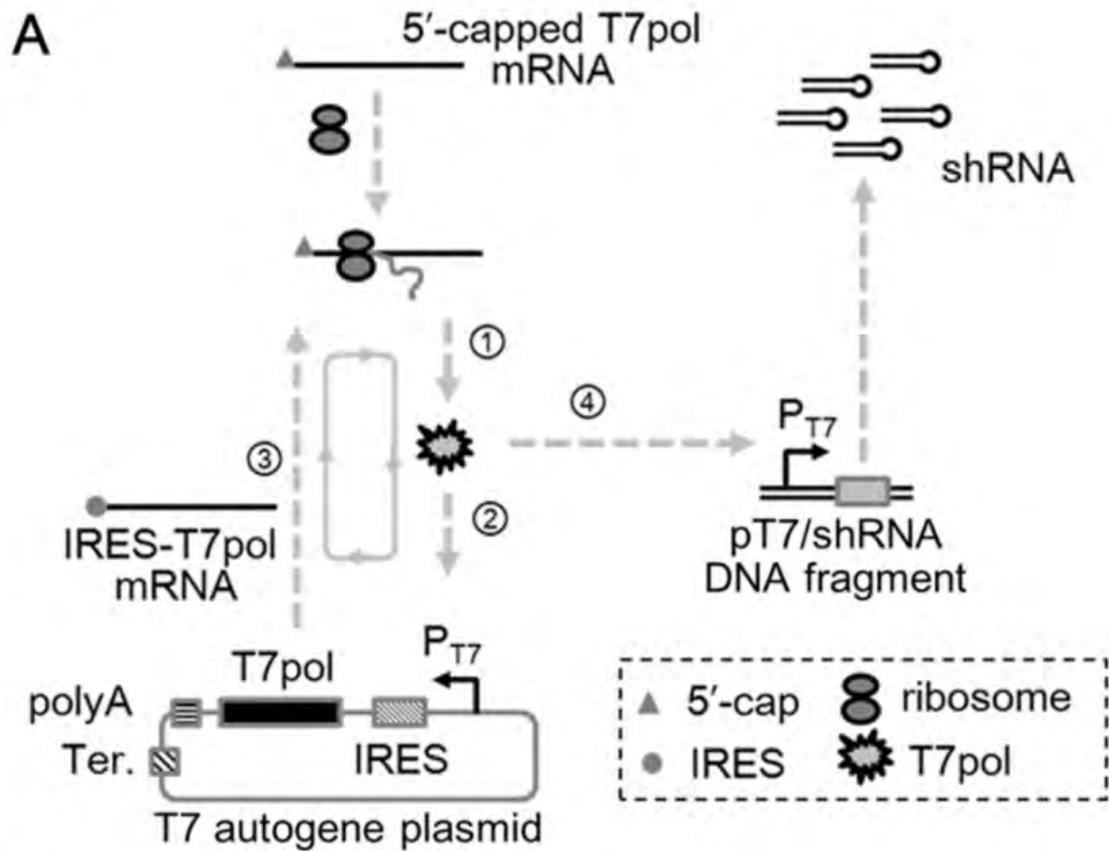
Exhibition Hall 2, FRI 11:00~12:30

A T7 autogene-based hybrid mRNA/DNA system for long-term shRNA expression in cytoplasm without inefficient nuclear entry

Hyung Jun Ahn

Center for Theragnosis, Korea Institute of Science and Technology, Korea

The transient silencing effects currently demonstrated by nonviral siRNA delivery systems limit the therapeutic utility of RNAi, but it remains a technical challenge to prolong duration of gene silencing. We have developed a T7 autogene-based hybrid mRNA/DNA system to enable long-term expression of shRNA in cytoplasm *in vitro* and *in vivo*. This hybrid mRNA/DNA system consists of T7 polymerase (T7pol) mRNA, pT7/shRNA-encoding DNA fragment and T7 autogene plasmid, and it can generate higher levels of T7pol proteins, compared to pCMV-triggering T7 autogene system, especially without the need of nuclear entry of any gene. A large amount of T7pol proteins produced are used to induce pT7-driven expression of shRNA in cytoplasm, and through cellular processing of RNA hairpins, mature siRNAs are generated for more than 13 days. We here demonstrate that a single liposomal delivery of this hybrid system leads to the long-term silencing effects *in vitro* and *in vivo*, in contrast to the conventional siRNA methods relying on the repeated administrations every 2 or 3 days. These sustainable shRNA expression properties in cytoplasm can provide an efficient strategy to address the limitations caused by shRNA-encoding plasmid DNA systems such as low nuclear entry efficiency and short-term silencing effect. The development of long-term shRNA expression system *in vivo* could scale down administration frequency of RNAi therapeutics in the treatment of chronic diseases, thereby increasing its clinical utility.



Poster Presentation : **LIFE.P-359**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Extracellular matrix delivery for tissue regeneration

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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 (HNDF) was 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, with 1.42 ± 0.11 times faster than 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.

Poster Presentation : **LIFE.P-360**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Multi-component Extracellular Matrix (ECM) Formation for 3D Cell Culture

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Extracellular matrix (ECM) protein networks provide microenvironment which determine cell differentiation, proliferation, signalling and molecular pathway. By using ECM network, 3D cell culture is feasible to be generated to mimic in vivo cellular behaviour. However, the architecture and chemical components are greatly variable and tissue specific. In this study, we applied microcontact printing of fibronectin as a template of controllable cellular fibronectin network formation for 3D cell culture application. We fabricated micro contact printing of fibronectin and cultured fibroblast on it. The FN patterned network then decellularized by freeze thawing method. Finally, the cells was reseeded on FN network and this step is repeated until several layers of cells grow on the FN-FN network specifically. Our method succesfully generated controllable FN-FN network from cells. Patterned FN-FN network then reseeded by second layer of fibroblast and maintain its viability for more than two weeks. Therefore, this ECM network has high potency to be applied for in vivo mimicking cell culture. Keywords: fibronectin, ECM, microcontact printing, 3D cell culture

Poster Presentation : **LIFE.P-361**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of HSP90 β Proteolysis Targeting Chimera (PROTAC) Protein Degradator

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In general, therapeutic strategies focus on the use of small molecules to influence the activity of disease-related proteins. However, there is an increasing demand for the development of new approaches to overcome the limitations of previously developed drugs as well as in the treatment of "undruggable targets". Here, a new concept coined PROTAC that aims to selectively induce proteolytic degradation of disease-related proteins is presented. The 26S proteasome is the main pathway for regulated degradation of cellular proteins in all eukaryotic organisms. The high specificity of the 26S proteasome is attributed to the ubiquitin (UB) pathway, thus for a protein to be degraded it must be ubiquitylated. The sequential action of three enzymes E1 (UB-activating), E2 (UB-conjugating), and E3 (UB-ligases) are necessary to attach UB to a target protein. Our strategy involves the recruitment of E3 to tag a specific target protein for degradation by the 26S proteasome. To achieve this, a molecular probe comprising a known E3 ligand tethered to a target specific ligand is constructed. Heat shock protein 90 (HSP90), involved in the division and survival of cancer cells was selected as the target of interest. Typical HSP90 inhibitors bind to the ATP-binding domain and affects the HSP90 chaperone cycling. However, the therapeutic application of HSP90 drugs are hampered due to solubility and hepatotoxicity issues. It is believed that the here presented PROTAC technology is a good alternative to selectively degrade HSP90 and is a viable new therapeutic approach.

Poster Presentation : **LIFE.P-362**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Structural basis for low catalytic activities in the two minor beta-carbonic anhydrases from the filamentous fungi *Aspergillus fumigatus*

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In the fungal kingdom, the beta-carbonic anhydrases (beta-CAs) are widely distributed zinc-metalloenzymes that play essential roles in growth, survival, development and virulence. In particular, the majority of filamentous ascomycetes possess multiple beta-CA isoforms in which the majors and minors have been characterized. Herein, we tested *in vitro* catalytic behaviors of the two minor beta-CAs, CafC and CafD, from *Aspergillus fumigatus*, and confirmed that both enzymes exhibit low CO₂ hydration activities. To understand the structural basis of their low activities, we further performed X-ray crystallographic and site-directed mutagenesis studies. Both enzymes exist as homodimer. Similar to other Type-I beta-CAs, CafC active site reveals the “open” conformation in which the zinc ion is tetrahedrally coordinated by three residues (C36, H88 and C91) and a water molecule. However, L25 and L78 on the rim of the catalytic entry site protrude into the active site cleft, partially occluding access to it. Consistent with our structural analysis, single (L25G or L78G) and double mutants provide functional evidences that widening the entrance to the active site greatly accelerates the catalytic reaction. By contrast, CafD shows a typical Type-II “closed” conformation in which a zinc-bound water is replaced by aspartic acid (D36). The most likely explanation of this result is that a completely conserved arginine is substituted to glycine (G38), therefore, D36 is not allowed to undergo a conformational change by forming a D-R pair that can leave a space for a zinc-bound water and switch the enzyme to be active. Furthermore, CafD structure reveals the presence of a copper ion in the interface, which may contribute to stabilize the dimeric assembly.

Poster Presentation : **LIFE.P-363**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhancement antigen binding affinity of scFv-protein nanocage with SpyCatcher/SpyTag system

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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 PDHs fused to SpyTag and scFv fused to SpyCatcher in E. coli. 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-364**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Identification of protein tyrosine phosphatase 1B inhibitors as antidiabetic drugs

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Insulin resistance is a key feature of type 2 diabetes and is characterized by downregulation insulin signaling. Protein-Tyrosine Phosphatase 1B (PTP1B) is a negative regulator of the insulin signaling pathways and its increased expression and activity lead to insulin resistance relevant to development of type 2 diabetes. Therefore, PTP1B inhibition is expected to be a potential therapeutic strategy to treat type 2 diabetes. In this study, we investigated whether six natural compounds may have an antidiabetic effect via a PTP1B inhibition. To identify therapeutic candidates for the treatment of type 2 diabetes, six natural compounds were screened for inhibitors of PTP1B relevant to cellular insulin resistance, measuring the enzymatic activity of PTP1B *in vitro*. Among them, SO48 and SO82 were selected as PTP1B inhibitors and we examined its IC_{50} , K_i value and inhibition type through enzyme kinetics. We also investigated the antidiabetic properties of PTP1B inhibitors in C2C12 muscle cells and 3T3-L1 adipocytes. Our cell-based studies demonstrated that SO48 and SO82 as PTP1B inhibitors could be used as a potential therapeutic candidate for the treatment of type 2 diabetes.

Poster Presentation : **LIFE.P-365**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Structure, Dynamics, and Hyperthermostability of Acyl Carrier Protein from *Thermotoga maritima*

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The acyl carrier protein from a hyperthermophile, *Thermotoga maritima*, was revealed to be extraordinary thermostable, allowing this protein to act as a carrier in the fatty acid synthesis (FAS) at extremely high temperature, higher than 80°C. To understand the key factors for the thermostability, the structure and dynamic features of the hyperthermophilic ACP (*Tm*-ACP) was investigated by NMR spectroscopy. The long $\alpha_1\alpha_2$ loop of *Tm*-ACP is stabilized by several hydrophilic and hydrophobic noncovalent interactions. Furthermore, an extensive ion cluster provides structural rigidity on the $\alpha_2\alpha_3$ loop, keeping hydrophobic cavity open and expanded compared to its mesophilic homologues. This important feature compensates the rigidity to shuttle acyl chains to FAS enzymes even at high temperature.

Poster Presentation : **LIFE.P-366**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

12-meric promising novel peptide antibiotic candidate for the treatment of Gram-negative sepsis

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Papiliocin, isolated from the swallowtail butterfly *Papilio Xuthus*, shows low toxicity and high bacterial cell selectivity particularly against Gram negative bacteria. Tertiary structures have revealed that these residues are composed of an N-terminal amphipathic α -helix and a hydrophobic C-terminal α -helix linked by a hinge. We determined the essential length of the N-terminal fragment of papiliocin necessary to retain its biological activity. The minimum inhibitory concentration values and cytotoxicity measurement revealed that a PapN-12mer containing a three-turn, amphipathic helix was the shortest peptide exhibiting antibacterial activity without cytotoxicity. Based on these results, we designed 12mer peptides derived from original sequence, to obtain more potent activity against multidrug resistant Gram-negative bacteria and to improve cell selectivity and anti-inflammatory properties. In a mouse sepsis model, especially, Pap12-6 significantly improved survival, reduced bacterial growth in organs, and reduced LPS and inflammatory cytokine levels in the serum and organs. Pap12-6 showed minimal cytotoxicity towards mammalian cells and controlled liver and kidney damage, proving its high bacterial selectivity. Our results suggest that Pap12-6 is a promising peptide antibiotic for the therapeutic treatment of Gram-negative sepsis via dual bactericidal and immunomodulatory effects on the host

Poster Presentation : **LIFE.P-367**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Psychrophilic Cold Shock Protein has Tyrosine in its Hydrophobic Core: Key Determinant of the Low Thermostability

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Cold shock proteins (Csp) function as RNA chaperones at lower-than-optimum temperatures. Here, we investigated the structure and dynamics of the psychrophilic Csp from *Colwellia psychrerythraea* 34H (*Cp*-Csp) for the first time. Despite of high sequence homology, its thermostability (37 °C) was markedly lower than those of other Csp. NMR spectroscopic analysis revealed that *Cp*-Csp has a flexible structure with only one salt bridge and 10 residues in the hydrophobic cavity. Instead of the conserved Phe, *Cp*-Csp contains Tyr51 in its hydrophobic core. The Y51F mutation increased the stability of hydrophobic packing and may have allowed the formation of a K3–E21 salt bridge, increasing the thermostability to 43 °C. *Cp*-Csp exhibited conformational exchanges in its ribonucleoprotein motifs 1 and 2, and these motions were decreased by the nucleic acid binding. Fewer salt bridges, longer flexible loops, and less compact hydrophobic cavity lead to the low thermostability of *Cp*-Csp. The conformational flexibility of *Cp*-Csp facilitates its accommodation of nucleic acids at low temperatures in polar oceans and its function as an RNA chaperone for cold adaptation.

Poster Presentation : **LIFE.P-368**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Natural TLR2 antagonist phloretin suppresses TLR2-mediated Inflammation

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Phloretin is a naturally occurring dietary flavonoid that is abundant in fruit. Here, we investigated whether the anti-inflammatory activity of phloretin is mediated through TLR2 pathways, and whether phloretin acts as an inhibitor of TLR2/1 heterodimerization. We tested the effects of phloretin on TNF- α production induced by various TLR-specific agonists. Phloretin significantly inhibited Pam3CSK4-induced signaling in Raw264.7 cells compared to TLR signaling induced by the other agonists tested. We further tested the effects of phloretin in HEK293-hTLR2 cells induced by Pam3CSK4, and confirmed that phloretin has comparable inhibition of TLR2/1 heterodimerization. Moreover, phloretin reduced the secretion of the inflammatory cytokines TNF- α and IL-8, whereas it did not significantly reduce these cytokines in cells. Western blot results showed that phloretin significantly suppressed Pam3CSK4-induced and NF- κ B p65 expression. The molecular interactions between phloretin and TLR2 were investigated using bio-layer interferometry and in silico docking. Phloretin bound with micromolar binding affinity, and we proposed a binding model of phloretin at the TLR2-TLR1 interface. Overall, we confirmed that phloretin inhibits the heterodimerization of TLR2/1, highlighting TLR2 signaling as a therapeutic target for treating TLR2-mediated inflammatory immune diseases.

Poster Presentation : **LIFE.P-369**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of a real-time FRET detection system for amyloid- β plaque formation towards therapeutic treatment of Alzheimer disease.

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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 unnatural fluorescent amino acid. But using dye with short wavelength range, interference may occur, so we used dye which are long wavelength band. In our design, a C-terminal FITC residue of the amyloid- β fragment act as the FRET donor to the Rhodamine b residue. However, only upon aggregation of the construct, the FRET pair is in close proximity to allow energy transfer. Consequently, excitation at 490 nm (i.e., FITC excitation maximum) results in significant sensitized emission at 580 nm (i.e., Rhodamine b emission maximum) 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 : **LIFE.P-370**

Life Chemistry

Exhibition Hall 2, FRI 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).

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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 or hypoxia, 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 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. 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, by either inducing or inhibiting apoptosis. 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. Generally, the label-free detection probe emits the strong signal when target protein which is a tryptophan and a probe is closed. In this system, the phase of MDM2 or Bcl-2 with tryptophan and a probe is affected energy transfer efficiency. So, changing of florescent intensity give us the information which is the binding conformation & affinity of MDM2 or Bcl-2 toward the probe. The label free FRET-based probe can be used as a tool for novel drug screening of MDM2 and Bcl-2 oncogenic proteins.

Poster Presentation : **LIFE.P-371**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Identification of Polyphyllin D as a Selective Inhibitor of SHP2 Against the Non Receptor PTPs

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SHP2 (encoded by the PTPN11) has an important role in signal transduction downstream of receptor tyrosine kinase. Activating mutation or overexpression of SHP2 have been reported in various types of human leukemia cancer such as Noonan syndrome, Acute Myeloid Leukemia (AML), Acute Lymphoid Leukemia (ALL). SHP2 promotes the activation of RAS. And is regulates cell survival and proliferation primarily through activation of ERK, AKT by regulating upstream of RAS. Recently, it is known as important mediator of immune checkpoint pathways. In brief, If SHP2 inhibitor apply to RAS-ERK associated disease that will be promise drug candidate for cancer. 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 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 ($K_i = 64.2 \mu\text{M}$). Furthermore, SHP2 inhibitor induce stronger cancer cell apoptosis in the signal associated with ERK, AKT and Bcl2. Together, these data demonstrate that efficacy of SHP2 inhibition is a valid therapeutic approach for the treatment of leukemia cancers.

Poster Presentation : **LIFE.P-372**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Amyloid fibril formation of fusion protein (ERLBD302-552-L23- α Syn) in the presence of ERLBD ligands

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In the brain of patients with Parkinson's disease, α -Synuclein (α Syn) protein forms amyloid fibrils. We previously examined the formation of α Syn amyloid in the presence of ERLBD ligand through ThT assay. In the present study, we studied the fibril formation of fusion proteins in which the ERLBD302-552 domain and α Syn were connected by a proper length of linker, L23. We successfully expressed and purified the fusion protein (ERLBD302-552-L23- α Syn) by affinity Ni²⁺-column purification. The amyloid formation process of fusion proteins was studied through ThT assay in the presence of ligands. Finally, photo-degradation of the fusion protein by the synthesized hybrid ligand was observed.

Poster Presentation : **LIFE.P-373**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The Structure and Substrate Specificity of *Propionibacterium acnes* β -ketoacyl Acyl Carrier Protein Synthase III

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Propionibacterium acnes is an anaerobic gram-positive bacterium found in the niche of the sebaceous glands in the human skin, and is a causal pathogen of inflammatory skin diseases as well as periprosthetic joint infection. To gain effective control of *P. acnes*, a deeper understanding of the cellular metabolism mechanism involved in its ability to reside in this unique environment is needed. *P. acnes* exhibits typical cell membrane features of gram-positive bacteria, such as control of membrane fluidity by branched-chain fatty acids (BCFAs). Branching at the iso- or anteiso- position is achieved by incorporation of isobutyryl- or 2-methyl-butyryl-CoA via β -ketoacyl acyl carrier protein synthase III (KAS III) from fatty acid synthesis. Here, we determined the crystal structure of *P. acnes* KAS III (*PaKAS* III) at the resolution of 1.9 Å for the first time. Conformation-sensitive urea polyacrylamide gel electrophoresis and tryptophan fluorescence quenching experiments confirmed that *PaKAS* III prefers isobutyryl-CoA as the acetyl-CoA, and the unique shape of the active site cavity complies with incorporation of branched-short chain CoAs. The determined structure clearly illustrates how BCFA synthesis is achieved in *P. acnes*. Moreover, the unique shape of the cavity required for the branched-chain primer can be invaluable in designing novel inhibitors of *PaKAS* III and developing new specifically targeted antibiotics.

Poster Presentation : **LIFE.P-374**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Hypoxia-Triggered Transforming Immunomodulator for Cancer Immunotherapy *via* Photodynamically Assisted Antigen Presentation of Dendritic Cell

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Recent tendency of cancer therapy is focused on immunotherapy as an alternative method. In spite of its strong anticancer effect, it has been reported that the immunoediting of cancer is an obstacle for successful immunotherapy. Among the pathways of immunoediting, the continuous mutation induces the heterogeneity of cancer, providing with a means of escape from attack of tumor-specific T cells. However, recent researches have demonstrated that cancer with high mutation rate showed valid therapeutic effect after cancer immunotherapy due to generation of neoantigens. Therefore, a direct release of endogenous tumor antigens from tumor cell itself can be a promising strategy for activation of anti-immune response despite of immunoediting. Herein, we reported a nanoparticle-based system for combinatorial anticancer therapy by introduction of photodynamic effect into immunotherapy. First, we have fabricated a MSN based nanoparticle whose surface covered with hypoxia-cleavable PEG for enhanced delivery of photosensitizer and adjuvant. The results from tumor infiltrated lymphocyte analysis showed that enriched dendritic cell population at tumor site after photodynamic therapy. Also, the hypoxia-responsible delivery of adjuvants and the release of tumor proteins induced by photodynamic effect results in increase of antigen presentations of the model tumor proteins, showing significant anti-tumor therapeutic effect in tumor regression study in vivo. Taken all together, the application of photodynamic therapy into immunotherapy is promising as recruiting dendritic cells and enhances antigen presentation process

Poster Presentation : **LIFE.P-375**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Purification and identification anti-inflammatory peptides derived from tIK derivatives

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RA is a severe autoimmune disease joint inflammation and the formation pannus tissue due to the synovial hyperplasia, which causes pro-inflammatory cells and macrophages for the destruction of cartilage and bone. Moreover, it is known that the disease is caused by an imbalance of pro-inflammatory cytokines and anti-inflammatory cytokines. But, recent studies have showed that truncated IK (tIK), which lacks the 315-amino acid sequence from the N - terminus, 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 bound to the Interleukin 10 receptor subunit alpha (IL-10RA) and had the same effect as the anti-inflammatory cytokine IL-10 that plays a potent treatment by inhibiting immune cells and deactivating macrophages. 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 that can calculate the distance between IL-10 and IL-10RA. Based on these results, we selected four epitopes that could have anti-inflammatory activity in tIK and selected the best anti-inflammatory peptide (tIK-YK4) using TH17 cell differentiation test. The peptide was re-truncated to 9-mer and 14-mer to confirm anti-inflammatory activity. Currently, we have successfully performed overexpression using E. coli and are optimizing the purification process. Finally, using purified peptides, we will identify the relationship between anti-inflammatory activity and structure.

Poster Presentation : **LIFE.P-376**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Antidiabetic effect of DH049 via inhibition of the protein tyrosine phosphatase PTPN11

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Tyrosine-protein phosphatase non-receptor type 11 (PTPN11), a member of the protein tyrosine phosphatase (PTP) family, PTPN11 is a cytoplasmic enzyme widely expressed in various tissues and cells. PTPN11 involved in the tyrosine kinase receptor signaling (EGF, insulin, etc.) stimulates RAS-RAF-MAPK and PI3K/AKT signaling pathway. The alteration of PTPN11 activity leads to abnormal development, tumorigenesis, and metabolic disease. In this study, we have screened natural compounds to identify potent inhibitors of PTPN11. Among them, DH049 was selected as a targeting inhibitor of PTPN11. We examined its K_i value and inhibition type *in vitro* and investigated the antidiabetic effect of DH049 in 3T3-L1 cells. Thus, these results suggest a valid therapeutic approach for the treatment of diabetes.

Poster Presentation : **LIFE.P-377**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of Selective S1P1 Receptor Agonists for Treatment of Multiple Sclerosis

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Multiple Sclerosis(MS) is an neurodegenerative autoimmune disorder of the central nervous system. The FDA-approved Fingolimod is the first oral drug for relapsing forms of MS. Following phosphorylation in vivo, an active form of fingolimod, acts as a sphingosine 1-phosphate(S1P) receptor modulator, binding with high affinity to S1P receptors(S1P1,3~5). Fingolimod causes many side effects such as bradycardia, hypertension, skin cancer, and macular edema due to non-selective binding. As a cause of bradycardia, a GIRK channel activated by G protein pathway signaling due to binding with S1P1 was suggested. The need for the development of S1P1 receptors which act as a β -arrestin pathway, has been suggested in order to avoid side effects caused by the G protein pathway. A total of 33 compounds were synthesized using five schemes, and Ca²⁺, β -arrestin and internalization assays were performed. Compounds that show efficacy as therapeutic agents have not been elucidated, but will be used to discuss and improve the results.

Poster Presentation : **LIFE.P-378**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of all cases of caffeoylquinic acid via protected quinic acid

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Caffeoylquinic acids (CQAs) was reported that have various biological activities including antioxidant, antibacterial, anticancer, and others. (-)- Quinic acid has four hydroxyl group and selective hydroxyl group protection in poly hydroxyl molecules continues to be a challenge in synthetic chemistry. In this study, a total 15 compounds were synthesized that combine one caffeic acid, two caffeic acid, three caffeic acid and four caffeic acid in (-)-quinic acid by selectively protecting the hydroxyl group. Furthermore, the compounds that I synthesized will treat specific cells to find out any other biological activity and which hydroxyl group is active.

Poster Presentation : **LIFE.P-379**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and structural investigation of cyclosporin O derivatives and its structure-permeability relationship (SPR) study

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As inspired by cyclosporin A (CsA) which was well known natural cyclic peptide with highly oral bioavailability, cyclic peptides have been widely discussed as a promising macrocyclic scaffold which possessed high permeability with large surface area and constrained conformation. Recently, unique structural features (e.g., N-methylation) and conformational changes depending on environmental polarity (chameleonicity) make cyclic peptides permeable was reported. In cyclosporine family, cyclosporin O (CsO) is a unique member in the absence of MeBmt residue which caused non-specific cyclophilin-binding and synthetic difficulty was adopted as a basic scaffold to design CsO derivatives. CsO and its derivatives were synthesized, and their structural investigation was carried out via NMR spectroscopy, computational calculation containing molecular dynamics and quantum mechanics. CsO exhibited transannular interactions as shown in CsA, while CsO derivatives demonstrated a modulated rigidity depending on specific substitutions. In addition, strength and exposure index toward solvent of hydrogen bonds were investigated to evaluate the conformational changes by environmental polarity. Under structural understanding, PAMPA and caco-2 permeability assay were carried out to investigate a structure-permeability relationship (SPR) of CsO derivatives. This study will provide a rationale design of cyclic peptides with more permeable and predictable physico-chemical properties.

Poster Presentation : **LIFE.P-380**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Metalloporphyrin-peptoid conjugates (MPPCs): Host-guest interaction and chiral recognition

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Natural heme cofactors utilize additional axial ligands such as methionine and histidine to finely control molecular energy level and geometry of metal center. By mimicking this interesting phenomenon and by introducing cooperativity to this natural strategy, porphyrin tweezers were developed as molecular tweezers for the analysis of chirality of substrates in the field of host-guest chemistry. However, porphyrin tweezers employing sequence-specific scaffold have rarely developed, although there is an anticipation to expand the application area of porphyrin tweezers including photo-, asymmetric, and oxidation catalysis. Herein, we synthesized metalloporphyrin-peptoid conjugates (MPPCs) displaying two metalloporphyrins on a peptoid scaffold with either achiral unfolded (1) or chirally helical (2 and 3) secondary structures. Host-guest complexation of MPPCs was realized with various guests of different lengths and basicities, and the extent of complexation was measured by UV-vis and circular dichroism (CD) spectroscopic titration. Based on this analysis, we can conclude that due to the inherent flexibility of peptoid backbone, MPPCs can recognize, contrast, and analyze various achiral, chiral, or racemic molecules possessing a broad type of functional groups. Currently, we are focusing to apply the host-guest complexation of MPPCs into a novel approach to control catalysis mediated by metalloporphyrins.

Poster Presentation : **LIFE.P-381**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Structural insights into catalytic mechanisms of the two major beta \square -carbonic anhydrases from the fungal pathogen *Aspergillus fumigatus*

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In fungi, the beta-class of carbonic anhydrases (beta-CAs) are ubiquitous zinc metalloenzymes that are essential for their growth, survival, differentiation, and virulence. Here we report the crystal structures and biochemical characterization of two tetrameric beta-CAs, CafA and CafB, from *Aspergillus fumigatus*, known as the major cause of invasive aspergillosis. Both enzymes exhibit apparent in vitro CO₂ hydration activity. Despite the overall similarities in structures, there are notable differences in the catalytic active sites. In CafA, the zinc ion is tetrahedrally coordinated by the three conserved residues (C119, H175, and C178) and a hydrated carbon dioxide (bicarbonate), indicating that it has “open” conformation (Type-I class). In contrast, CafB shows novel active site in which the disulfide bond formation between zinc-ligating two cysteines (C57 and C116) expels the zinc ion, and closes the active site incapable of binding a substrate. Site-directed mutagenesis represents a potential role of Y159 as a proton-coupled electron transfer during oxidative inactivation. CafB also has a non-catalytic (inhibitory) site for bicarbonate binding to regulate its activity allosterically. Our results suggest that the two closely related CafA and CafB utilize the different types of catalytic mechanisms; CafA is active in a broad range of pH, but CafB is subject to oxidative inactivation and/or allosteric substrate inhibition. *A. fumigatus* may use this sophisticated activity-withholding strategy to enhance survival capacity in the infected human.

Poster Presentation : **LIFE.P-382**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Histidine-containing antimicrobial peptoids

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Antimicrobial peptides (AMPs) are one of the promising antibacterial therapeutic agents, however, despite the activity against broad spectrum pathogens, several drawbacks such as salt sensitivity, rapid degradation, and cost problem are still remained as unresolved tasks. Interestingly, salt resistance of some AMPs from marine organisms was reported, and the marine AMPs have been actively investigated to figure out properties and mechanisms. Especially, clavanins, piscidin, and chrysopsins which are known as histidine-rich marine AMPs show salt resistance and broad range activity against bacteria. Peptoids, *N*-substituted glycine polymers, which maintain sequence specificity and resistance to protease have been used in drug discovery to overcome previously mentioned disadvantages of AMPs. In this study, we designed and synthesized antimicrobial peptoid library which contained Mhis, *N*-(methylimidazole) glycine that mimics histidine. The α -helicity of each peptoids were analyzed by circular dichroism spectroscopy. The antimicrobial activity was determined by minimum inhibitory concentration (MIC) assay. Furthermore, these assays were performed in physiological salt conditions (150 mM NaCl) to examine salt resistance.

Poster Presentation : **LIFE.P-383**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Targeting NHR2 domain of AML1-ETO via bivalent peptides.

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AML (Acute Myeloid Leukemia), an aggressive cancer of the myeloid cells, makes up 32 % of all adult leukemia patients. One of the representative karyotypic abnormality for AMLs patients is translocation t(8;21)(q22;q22), which combines AML1 gene in chromosome 21 and ETO gene in chromosome 8. Expression of AML1-ETO fusionprotein, expressed through a result of the translocation t(8;21), is closely related to AMLs development. Unlike normal AML1, AML1-ETO act as a transcription factor that inhibits the transcription of hematopoiesis-related genes and blocks hematopoietic differentiation. As a result of the alternation of transcription activity, AML1-ETO leads leukemogenesis. Among the five domains of AML1-ETO, NHR2 domain plays an important role in protein-protein interaction to E protein families. Several studies approved that the inhibition of functions of NHR2 domain blocks leukemogenesis and inhibits proliferation of t(8;21) AML cancer cells. These studies shows that targeting NHR2 domain could be an interesting therapeutic strategy for modulating AMLs. Despite the importance of NHR2 domain, however, no inhibitors have been developed for controlling the PPI between NHR2 domain and E proteins. Here, we designed inhibitor for NHR2 domain to control protein-protein interaction between NHR2 domain and E proteins. The binding affinity between NHR2 domain and short N2B peptide, NHR2 binding domain of E protein, has been reported previously, however, the binding affinity was quite low (KD = 0.38 mM). Starting from the crystal structure, we designed NHR2 domain targeting bivalent peptides which various length of linker to obtain the maximal binding. Designed bivalent peptides showed 10-fold improved binding affinity compare to the monovalent N2B peptide. Designed peptides will serve as a useful chemical modulator to inhibit the function of NHR2 domain. And it will provides a promising starting point for the development of a novel class of therapeutic agents for AMLs. Reference[1] Nature, 2013, 500 (7460), pp 93-97.[2] ACS Med. Chem., 2013, 4 (3), pp 344-348.[3] J. Am. Chem. Soc, 2006, 128 (26), pp 8615-8625.

Poster Presentation : **LIFE.P-384**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Two Color, Cell-based on-bead Screening for Discovering Ligands of the Viral G Protein-Coupled Receptor

Junhyung Park, Hyun-Suk Lim^{1,*}

Division of Advanced Materials Science, Pohang University of Science and Technology, Korea

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

Herpesviruses family use their virally encoded GPCRs for viral pathogenesis. It is reported that Kaposi's sarcoma-associated herpesvirus (KSHV)-infected cells express the virally encoded GPCR. This viral GPCR is highly related to Kaposi's sarcoma which is the most frequent type of tumor that occurs in HIV-infected patients and remains a significant cause of death in AIDS sufferers.¹ Therefore, the viral KSHV GPCR is an attractive therapeutic target for the treatment of Kaposi's sarcoma. To develop the specific ligands to the GPCR, knowing crystal structure of GPCR can be an important reference. However, it is very challenging to crystallize the membrane protein due to its inherent instability if it is isolated from plasma membrane. These limitations can be addressed through the formation of chimeric construct with binding partners to stabilize the conformation of GPCR. Thus, discovering ligands for the target GPCR can be a good starting point for crystallization of GPCR as well as identifying ligands for GPCRs. In this regard, we discovered the ligands for the KSHV GPCR through two color, cell-based on-bead screening method without protein purification. In this method, target receptor expressing cell and parental cell that lacks the receptor of interest are labeled with different quantum dot respectively, which enables to select ligand that specifically binds to the target membrane protein. We used OBOC cyclic peptoid library for screening. Identified ligands is now being used for binding assay against the KSHV GPCR. References¹. Akrit Sodhi, Silvia Montaner, J. Silvio Gutkind*, *Nat. Rev. Mol. Cell. Biol.* 2004, 5, 988-1012

Poster Presentation : **LIFE.P-385**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Clustering Effect of Interleukin-1 Receptor Antagonist on the Ferritin Nanocage

Ga Hyeon Kim, Sang Jeon Chung^{1,*}

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¹*College of Pharmacy, SungKyunKwan University, Korea*

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-386**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Assessment of Cell Permeability of Bicyclic Peptoids

Wang Heemyeong, Hyun-Suk Lim*

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

Peptoids, oligomers of N-substituted glycines, are an attractive class of peptidomimetics with several desirable features such as ease of synthesis and proteolytic stability. Notably, it is well known that peptoids have better membrane permeability than native peptides. However, peptoids generally have relatively flexible structures, making it challenging for targeting intracellular proteins with high affinity and specificity. Macrocyclization has emerged as one strategy to solve these kinds of limitations. Macrocyclic peptoids are expected to have relatively rigid and preorganized structures compared to their linear counterparts, allowing them to bind more tightly to target proteins without major entropy penalty. Indeed, we recently demonstrated that monocyclic peptoids have better cell permeability compared to linear peptoids.¹ In addition, we previously developed highly efficient cyclization method for bicyclic peptoids which are expected to have improved conformational rigidity.² However, while the cell permeability of monocyclic peptoids was studied, that of bicyclic peptoids has not been explored yet. Herein, we evaluated the cell permeability of bicyclic peptoids through a systematic investigation method for cell penetration. Halotag-labeled linear and bicyclic peptoids were synthesized priorly, and their penetration was monitored by Confocal microscopy. As expected, bicyclic peptoids showed improved membrane permeability than their linear counterparts indicating that they will serve as potential protein capture agents given their excellent cell permeability in addition to their conformational rigidity and proteolytic stability. References 1. Shin, M. K.; Hyun, Y. J.; Lim, H. S. *ACS Comb. Sci.*, 2018, 20, 237-242. 2. Lee, J. H.; Kim, H. S.; Lim, H. S. *Org. Lett.* 2011, 13, 5012-5015.

Poster Presentation : **LIFE.P-387**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Conformational Studies of Cyclic α -ABpeptoids

Eun-Kyoung Jee, Hyun-Suk Lim*

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

Peptidomimetics foldamers that fold into well-defined conformations and incorporate diverse proteogenic and nonproteogenic side chains would be attractive alternatives to native peptides due to their proteolytic resistance. For a decade, many efforts have been made to develop diverse peptidomimetic foldamers. Among them, peptoids are a class of peptidomimetics based on N-alkylated glycines. They can be easily synthesized by solid-phase method, and have better cell permeability than native peptides and great potential to interrogate protein functions and therapeutic candidates. However, peptoids are relatively flexible and have difficulty in forming the folding structures because of the lack of backbone chirality. To address these limitations, we previously reported α -ABpeptoids (α -alkyl beta-peptoids) by inserting chiral methyl groups on carbonyl α -position. Although the CD spectra of α -ABpeptoids with various side chains showed folding conformations, their crystal structures have not been revealed yet. Macrocyclization is one of promising strategies to enhance conformational rigidity, therefore, it is considered that the possibility of forming crystal structures may be increased. Synthesized linear α -ABpeptoids in different lengths were macrocyclized and they have a characteristic CD spectra. Finally, the structure of cyclic α -ABpeptoid tetramer was solved through X-ray crystallography. It is the first time to confirm X-ray crystal structure of α -ABpeptoids.

Poster Presentation : **LIFE.P-388**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Comparison of Cell Permeability of α -ABpeptoids and Peptides

Min-Jae Kang, Hyun-Suk Lim*

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

Peptoids, oligomer of N-substituted glycine, are a class of peptidomimetics. They are easy to synthesize, resistant to proteolysis, and relatively cell permeable compared to natural peptides. However, peptoids are flexible and difficult to form secondary structures due to lack of chiral centers, which could limit the binding affinity with target proteins. Recently, we developed α -alkyl beta-peptoids (α -ABpeptoids), which have chiral methyl group at α position of the main chain to enhance the structural rigidity. As expected, α -ABpeptoids showed characteristic circular dichroism (CD) spectrum, which suggested that they form ordered conformations. α -ABpeptoids lack amide protons like peptoids, so they are expected to be cell permeable as much as peptoids. However, no systematic studies of cell permeability of α -ABpeptoids have been reported yet. Herein, we compared cell permeability of peptides and α -ABpeptoids having different lengths using cell penetration assay. α -ABpeptoids tend to have enhanced cell permeability compared to peptides by analyzing fluorescence-activated cell sorting and confocal microscopy. This implies that α -ABpeptoids could serve as a useful source of protein binding molecules, particularly targeting intracellular proteins.

Poster Presentation : **LIFE.P-389**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Spatiotemporal proximity crosslinking by light activation (Spot-light) reveals RNA processing machinery on the mitochondria in live cells.

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¹Department of Chemistry, Seoul National University, Korea

Proximity labeling is a recently developed method that enables proteomic profiling of specific regions in living cells. However, the diffusive character of in situ-generated reactive species by proximity labeling enzymes cannot be used easily to identify physically interacting partners with the protein of interest (POI). In the present study, we developed an in vivo proteome mapping method that enables spatiotemporal proximity crosslinking by a genetically targeted light-activated ligand of the HaloTag protein in a live mammalian cell (Spotlight). The spatiotemporally confined photo-crosslinking reaction at the surface of the HaloTag protein within the short lifetime of in situ generated nitrene ensures that the crosslinked product is a physically interacting protein of the POI. The specificity of this reaction was confirmed by selective capturing a rapamycin-induced protein interaction between FK506 binding protein (FKBP) and the FK506-rapamycin binding (FRB) domain in living cells. In addition, Spotlight was used to reveal the unknown interaction partner of a newly identified mitochondrial protein, exonuclease 3'-5' domain containing 2 (EXD2) in mammalian cells. From this experiment, A kinase anchoring protein 1 (AKAP1) was identified to be the major interacting partner of EXD2 at the outer mitochondrial membrane. This result illuminates that the biological function of EXD2 might be related to RNA processing on the mitochondrial surface. Overall, our results show that Spotlight can be a novel proteomic mapping tool to reveal the in vivo interactome of POI in living mammalian cells.

Poster Presentation : **LIFE.P-390**

Life Chemistry

Exhibition Hall 2, FRI 11:00~12:30

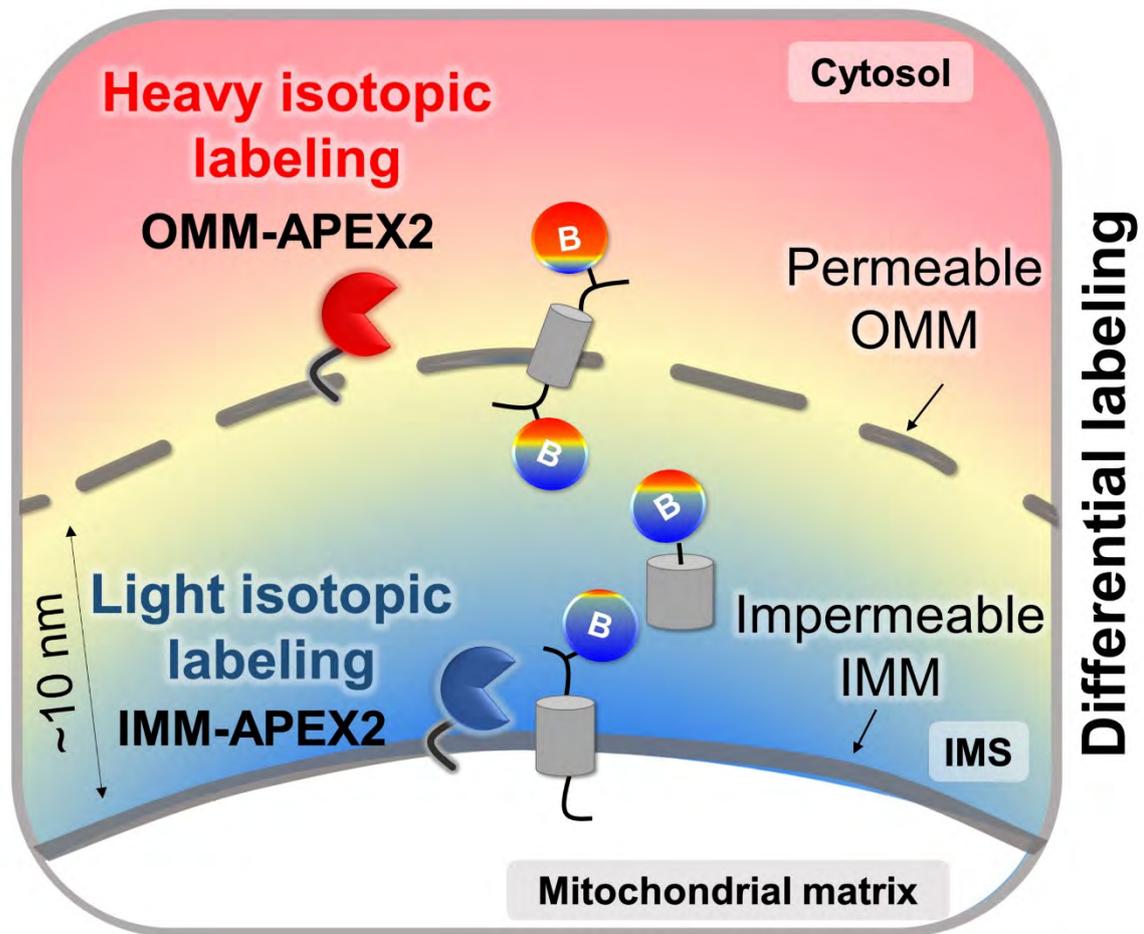
Global topology analysis of the permeable outer mitochondrial membrane by isotope-coded phenoxyl radical labeling in live cells

SongYi Lee, Jong-Seo Kim^{1,*}, Hyun-Woo Rhee*

Chemistry, Seoul National University, Korea

¹*Seoul National University, Korea*

Outer mitochondrial membrane (OMM) proteins play pivotal roles in the regulation of cell physiology. However, topological information for OMM proteins is lacking, in part because conventional methods cannot be applied to porous membranes. To unveil the architecture of the OMM proteome in live cells, we developed a new isotopic biotin-phenol probe and conducted a quantitative proteomic analysis of the intermembrane space and cytosol-facing tyrosine residues of OMM-localized proteins via direct mass spectrometric identification of the isotope-labeled peptides. Using this approach, we were able to clearly resolve the orientation of many OMM-associated proteins, including VDAC1 and PRDX1.



Poster Presentation : **ORGN.P-140**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Ferroelectric Switching Property of a 1,2,3-Triazole-based Helical Columnar Liquid Crystal

Byoung-Ki Cho*, **Manh Linh Nguyen**¹

Department of Chemistry, Dankook University, Korea

¹*Chemistry, Dankook University, Korea*

Recently, the ferroelectric columnar liquid crystals (LCs) have been drawing a great deal of attention due to its promising application as electronic materials. To pursue such LC materials, we speculated that the helical assembly and proper functional groups would be key factors. Here we designed a naphthalene derivative based on 1,2,3-triazolyl linkage through Click reaction because the resulting asymmetric triazole has structural rigidity and high dipole moment (4.55 Debye). The rotation of triazolyl group could result in two different cisoid and transoid conformation which have non-zero and zero dipole moments, respectively. As revealed by X-ray scattering and X-ray simulation, the molecules adopt the cisoid conformation to form a double-stranded helical columnar LC (Colhel) with a non-zero axial polarization. The homeotropic alignment could be done in both thin (5 μm) and bulk-level film (250 μm) on cooling from isotropic liquid phase (Liq) to Colhel under the application of an E-field. The switching experiments demonstrated the polar switching behavior in the temperature range from 105 to 115 oC. On the other hand, the ferroelectric switching was not observed at lower temperature Colhel such as 80 oC. This result can be explained by the weakening of H-bonding with increasing temperature. All details will be addressed in the poster presentation.

Poster Presentation : **ORGN.P-141**

Organic Chemistry

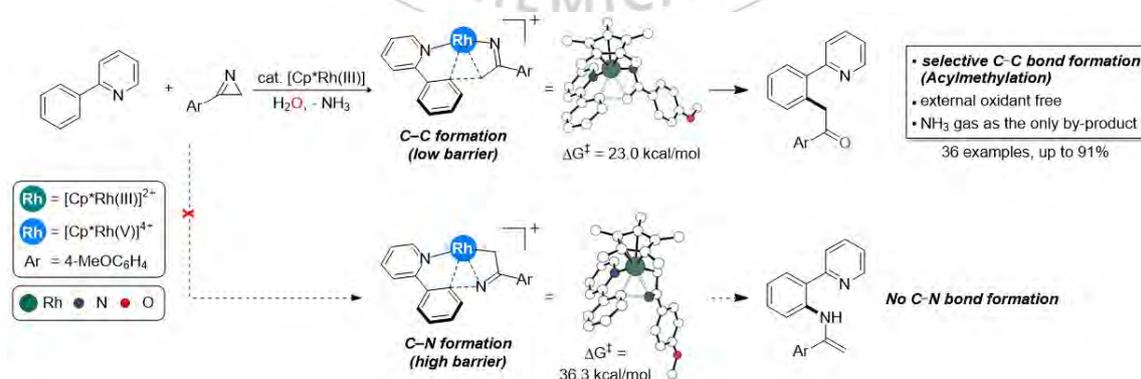
Exhibition Hall 2, THU 11:00~12:30

Selective C–C Bond Formation from Rhodium-Catalyzed C–H Activation Reaction of 2-Arylpyridines with 3-Aryl-2H-azirines

Sang Hoon Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

A novel method for the synthesis of acylmethyl-substituted 2-arylpyridine derivatives using 3-aryl-2H-azirines was developed by exploring a prototype reaction using DFT-calculations and carrying out targeted experiments guided by the calculated mechanism. 2H-Azirine was initially hypothesized to ring-open at the metal center to furnish familiar metal nitrene complexes that may undergo C–N coupling. Computational studies quickly revealed and prototype experimental work confirmed that neither the formation of the expected metal nitrene complexes nor the C–N coupling were viable. Instead, azirine ring-opening followed by C–C coupling was found to be much more favorable to give imines that readily underwent hydrolysis in aqueous conditions to form acylmethyl-substituted products. This new method was highly versatile and selective toward a wide range of substrates with high functional group tolerance. The utility of the new method is demonstrated by a convenient one-pot synthesis of biologically relevant heterocycles such as pyridoisindole and pyridoisquinoline.



Poster Presentation : **ORGN.P-142**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

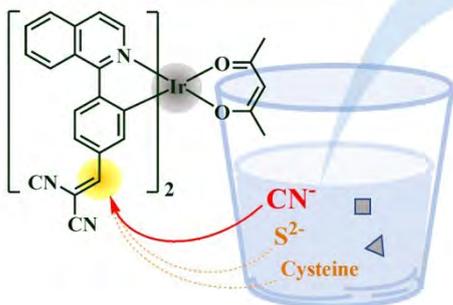
Potential-Dependent Electrochemiluminescence for Selective Molecular Sensing of Cyanide

Taemin Kim, Jong-in Hong*

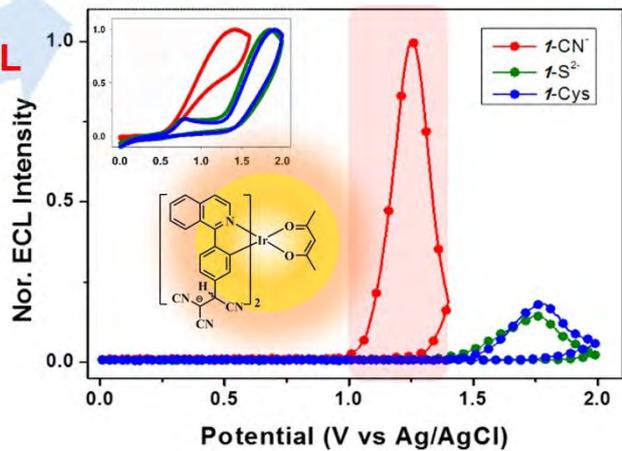
Division of Chemistry, Seoul National University, Korea

Although tremendous efforts have been devoted to providing specificity for molecular sensors, most of methods focus on structural variation of the binding or reaction site to improve selectivity. Herein, we report a new approach that a chemical probe, possessing a mediocre recognition site, can successfully discriminate a target among various interferences only with electrochemical manipulation. The dicyanovinyl group of the synthetic probe (1) was expected to react not only with a cyanide anion (CN^-), but also with sulfides and biothiols to produce similar adducts. However, the binding adduct (1-CN^-) between 1 and CN^- has significantly different energy levels to be only able to undergo electrochemical oxidation under ~ 1.0 V (vs. Ag/AgCl), which eventually generated strong electrochemiluminescence (ECL). The ECL emission from 1-CN^- can successfully discriminate CN^- without significant interferences from other analytes including sulfides and biothiols, and exhibited a linear correlation ($R_2 = 0.994$) with CN^- concentrations in a range of $0\text{--}400$ μM (LOD = 0.3 μM , $n = 5$). Energy density calculations were utilized to design the entire strategy, and electrochemical studies supported the mechanism of CN^- discrimination. Our approach was finally applied to direct trace analysis of CN^- in tap water (≥ 1 μM), and showed excellent performance suggesting a new, versatile, and rapid determination method for molecular toxins in real samples.

A probe with ordinary selectivity



Complete discrimination at 1.2 V



Poster Presentation : **ORGN.P-143**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Porphyrinoids Containing Exocyclic Double Bonds at meso-Positions: meso-Indanedionyl-dibenzihexaphyrins and Thia-(p-benzi)porphyrin

Chang Hee Lee^{*}, Seong-Jin Hong

Department of Chemistry, Kangwon National University, Korea

The novel meso-alkylidenyl porphyrinoids are non-aromatic and conformationally flexible macrocycles displaying unusual prototropy and unique protonation selectivity depending on the number of core-hydrogen. Most of the reported meso-alkylidenyl porphyrinoids displayed site-selective protonation and pyrrole inversion in some cases. For example, the compounds containing no core hydrogen are protonated at core nitrogen. However, the compounds bearing core-hydrogens are protonated at meso-(α)-position with concomitant hypsochromic shift of the absorption maxima. As a part of our endeavor for the construction of the new expanded porphyrinoid macrocycles, we have synthesized expanded meso-alkylidenyl dibenzihexaphyrins and fully characterized by ¹H NMR and HRMS spectroscopy as well as the single crystal X-ray diffraction analysis. The synthesis was accomplished by a typical '3+1' type of the mixed condensation. Synthesized compounds contain multiple exocyclic carbon-carbon double bonds at meso-positions. The p-benzihexaphyrin adopts two pyrroles inverted geometry with the intramolecular hydrogen bonding between pyrrolic N-H and carbonyl moiety of the indanedione. In case of m-benzihexaphyrin, the intermediate macrocycle bearing meso-hydroxy groups were isolated and characterized. The crystal structure analysis indicates that the molecules adopts *ci* symmetry with cylindrical shape through four intramolecular hydrogen bonding between pyrrole NHs and carbonyl group of indanedione. We carried out ¹H NMR spectroscopic studies in the presence of trifluoroacetic acid at elevated temperature. The appearance of a new resonance at 4.72 ppm indicates that protonation occurred at meso-□-positions. In this presentation, Synthesis, structural characteristics and protonation selectivity studies will be presented.

Poster Presentation : **ORGN.P-144**

Organic Chemistry

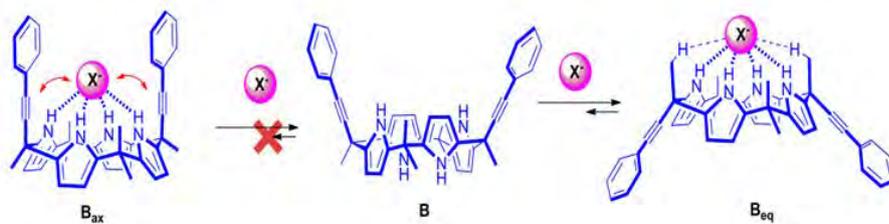
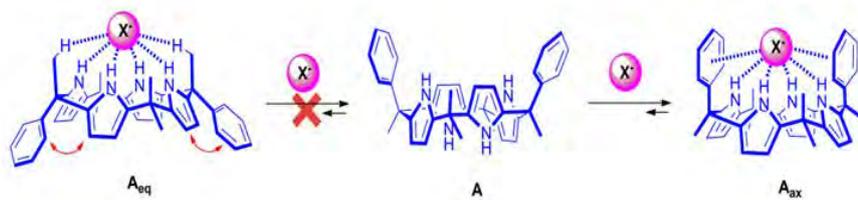
Exhibition Hall 2, THU 11:00~12:30

Anion-Alkyne Repulsion Regulates Anion Binding Domains in meso-bis-arylethynyl Calix[4]pyrroles

Chang Hee Lee*, **Ranjan Dutta**

Department of Chemistry, Kangwon National University, Korea

Functionalization of meso-positions of calix[4]pyrroles is the most viable strategy to design 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. Moreover, existence of attractive or repulsive interactions between the π -systems of installed meso-aryl groups and anions are well established with variety of model systems. 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 Meso-substituted calix[4]pyrroles containing direct meso-ethynyl linker displayed high binding affinities and unique conformational features on halide anion binding. A general conformational bias for the equatorial alignments of the meso-(aryl)ethynyl groups were observed in the host-halide complexes which was attributed to the repulsive anion-alkyne interactions and released steric strain. Synthetic details, conformational features and comparative halide anion binding properties will be presented.



Poster Presentation : **ORGN.P-145**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Blue Thermally Activated Delayed Fluorescence Emitters Using Modulated Triazine Electron Acceptors.

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Seoul National University, Korea

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

The development of organic light emitting diodes (OLEDs) for display devices has attracted significant attention over the past decade. In recent years, thermally activated delayed fluorescence (TADF) has attracted a lot of interest because TADF enables ultimate internal quantum efficiency (IQE) through reverse intersystem crossing (RISC) from the triplet state (T_1) to the singlet state (S_1). Nonetheless, in contrast to red and green emitters, blue emitters require a wide band gap, so only a few examples of blue TADF emitters have been reported. Herein, we report new blue TADF emitters using modulated triazine acceptors. These emitters showed high photoluminescence quantum yield (PLQY) and blue fluorescence in solution and doped film. The transient photoluminescence (PL) clearly showed both prompt PL and delayed PL, confirming that the emitters are able to harvest both singlet and triplet states. Details of synthesis, photophysical properties and device data will be presented.

Poster Presentation : **ORGN.P-146**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

BODIPY-Based Electrochemiluminescence Probes for Rapid Detection of Hydrogen Peroxide

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

Three BODIPY-based H₂O₂ probes were designed and synthesized. Among those probes, **2F** exhibited both the best stability during the ECL process and rapid detecting ability, which is highly promising for an ECL probe applied into point-of-care testing (POCT). Responses of the probes to H₂O₂ were examined in UV-vis/photoluminescence (PL)/ electrochemiluminescence (ECL) systems, suggesting that unsubstituted BODIPY causes deflation of ECL. Furthermore, the detection speeds of **2** and **2F** were compared in various pH conditions. **2F** performed an excellent detection of H₂O₂ with low detection limit and high selectivity.

Poster Presentation : **ORGN.P-147**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

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

¹*Department of Chemistry, Sogang University, Korea*

²*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

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.

KOREAN CHEMICAL SOCIETY

Poster Presentation : **ORGN.P-148**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

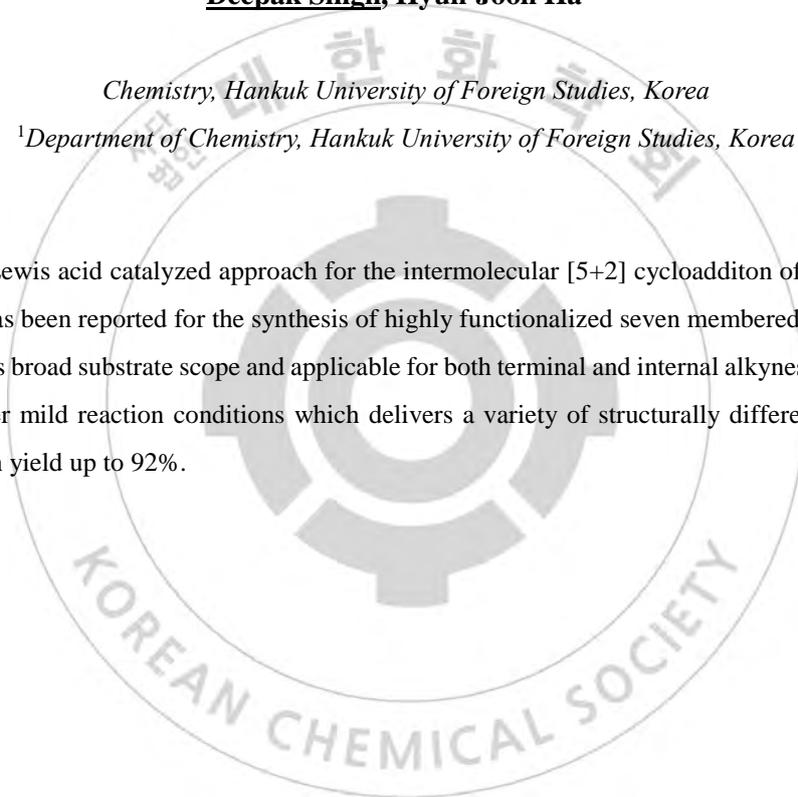
Metal-Free Aza-Claisen Type Ring Expansion of Vinyl Aziridines: An Expeditious Synthesis of Seven Membered N-Heterocycles

Deepak Singh, Hyun-Joon Ha^{1,*}

Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

A metal free, Lewis acid catalyzed approach for the intermolecular [5+2] cycloaddition of vinyl aziridines with alkynes has been reported for the synthesis of highly functionalized seven membered N-heterocycles. The method has broad substrate scope and applicable for both terminal and internal alkynes as well as vinyl aziridines under mild reaction conditions which delivers a variety of structurally different azepines ring systems in high yield up to 92%.



Poster Presentation : **ORGN.P-149**

Organic Chemistry

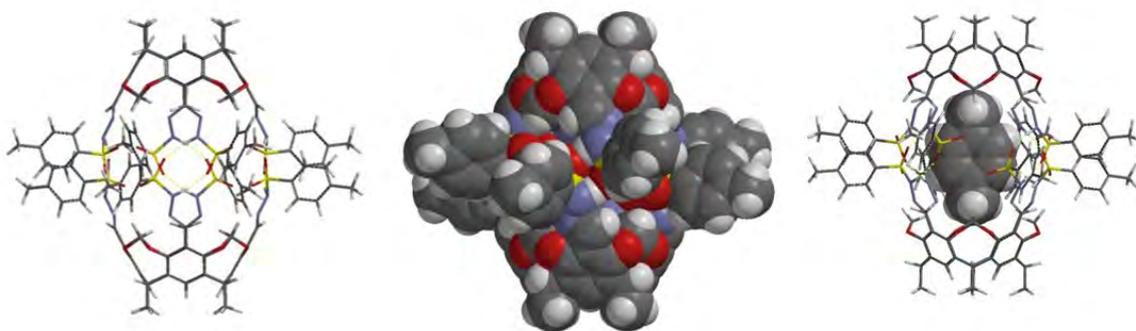
Exhibition Hall 2, THU 11:00~12:30

New self-assembled molecular capsule base on the hydrogen bonding of sulfonamido moiety

Yang Ryeong Kim, Yeon Sil Park, Kyungsoo Paek*

Department of Chemistry, Soongsil University, Korea

The self-assembled molecular capsules with an isolated nanospace are a very attractive area in supramolecular chemistry. Encapsulation of guest in the molecular capsules can be used for various applications such as sensing, catalysis, molecular storage and selective recognition. The hydrogen bonds have an advantage in the formation of self-assembled capsules because complementary functional groups such as urea, amide and imine would be directly associated with each other. Although, molecular capsules based on various complementary functional groups have been studied intensively, to our knowledge, a self-assembled capsule with sulfonamido group is without precedent. The new tetrakis(tolylsulfonamidoimino)-cavitand easily self-assembled with a suitable guest in non-polar solvents to give kinetically and thermodynamically stable molecular capsule, which was stabilized by the eight intermolecular sulfonamide $N-H \cdots O=S$ hydrogen bonds, two from each four paired sulfonamido moieties.



Poster Presentation : **ORGN.P-150**

Organic Chemistry

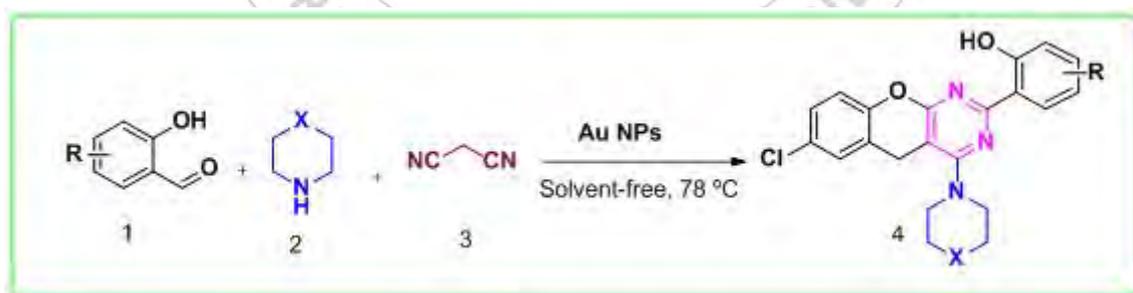
Exhibition Hall 2, THU 11:00~12:30

Green synthesis and characterization of gold nanoparticles (Au NPs) from extract of fruit *Schisandra chensis*: Catalytic activity studies towards the synthesis of chromeno[2,3-d]pyrimidin-2-yl)phenol derivatives

Sandip gangadhar Balwe, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

We have demonstrated a novel, facile, economic, and green synthetic protocol to produce gold nanoparticles (Au NPs) by using *Schisandra chensis* fruit extract. The synthesized Au NPs were characterized using UV–VIS spectroscopy, transmission electron microscopy, scanning electron microscopy, X-ray diffraction (XRD), FTIR, and energy dispersive X-ray analysis (EDXA). The catalytic efficiency of synthesized Au NPs were studied for one-pot construction of chromeno[2,3-d]pyrimidin-2-yl)phenol derivatives via one-pot three component reaction.



Poster Presentation : **ORGN.P-151**

Organic Chemistry

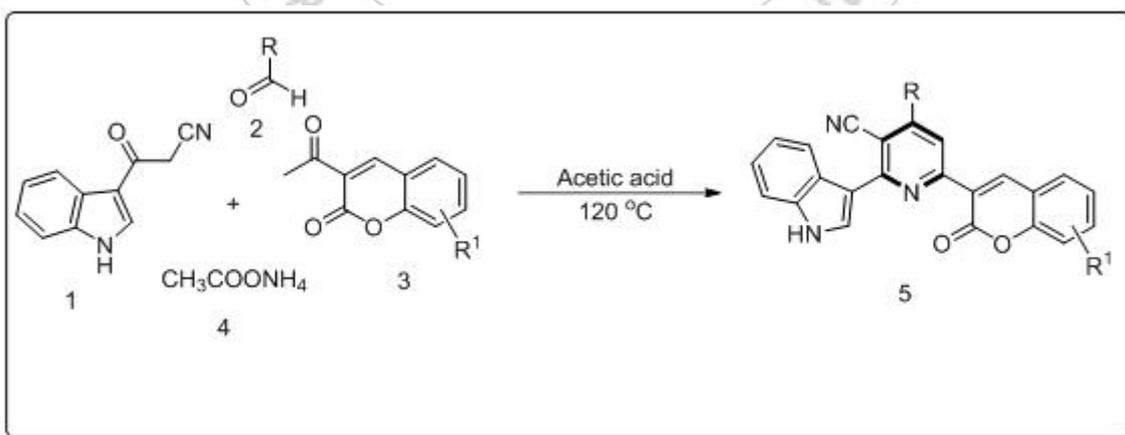
Exhibition Hall 2, THU 11:00~12:30

Acid-mediated one-pot four-component domino protocol for the construction new indole and coumarin containing pyridine-3-carbonitrile derivatives

Sandip gangadhar Balwe, Yeon Tae Jeong*, Maruti Yadav

Department of Display Engineering, Pukyong National University, Korea

A highly efficient one-pot domino protocol for the construction of novel indole and coumarin containing pyridine-3-carbonitrile derivatives has been described. The reaction proceeds via one-pot four-component condensation of 3-(1H-indol-3-yl)-3-oxopropanenitrile with various aromatic and aliphatic aldehydes, 3-acetyl-2H-chromenones and ammonium acetate in presence of acetic acid. The present new methodology offers several advantages such as short reaction time, easy experimental work-up, good yields and endures the substrate diversity, operational simplicity under metal-free reaction conditions for formation of C-C/C-N bonds.



Poster Presentation : **ORGN.P-152**

Organic Chemistry

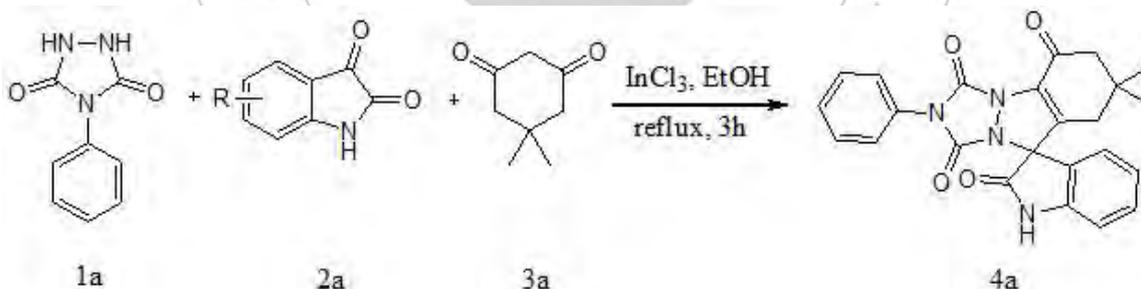
Exhibition Hall 2, THU 11:00~12:30

Indium chloride catalysed one-pot, three-component synthesis of spiro triazolo[1,2-a]indazole-tetraone derivatives

Amol Jadhav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

A mild, efficient, and expeditious method has been developed for the synthesis of spiro triazolo[1,2-a]indazole-tetraones via a one-pot three-component reaction of 4-Phenylurazole, isatins and cyclic-1,3-diketones in the presence of a catalytic amount of indium(III) chloride as a Lewis acid catalyst in ethanol at 80 °C conditions. The present protocol offers some advantages such as operational simplicity with easy workup, shorter reaction times, good to excellent yields with superior atom economy and environmentally benign reaction conditions.



Poster Presentation : **ORGN.P-153**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Water soluble Nano Particles for Effective Drug Delivery in Photodynamic Therapy

Yang Liu

Nano science and engineering, Inje University, Korea

Photodynamic therapy (PDT) is a treatment that uses a drug, called a photosensitizer or photosensitizing agent, and a particular type of light. When photosensitizers are exposed to a specific wavelength of light, they produce a form of oxygen that kills nearby cells. It has some advantages, such as: 1) It has no long-term side effects when used properly. 2) It's less invasive than surgery. 3) It usually takes only a short time and is most often done as an outpatient. 4) It can be targeted 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. More important thing is that the modified PS should be more soluble in water to get a balance for stability and reactivity. Our current work is focusing on improve the ps's water solubility by making them particle size.

Poster Presentation : **ORGN.P-154**

Organic Chemistry

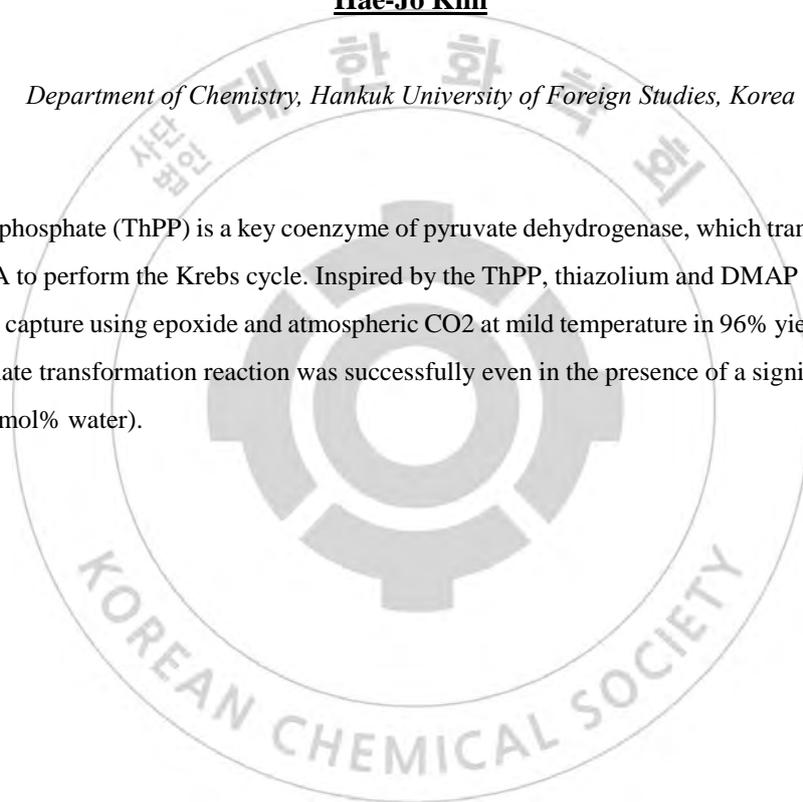
Exhibition Hall 2, THU 11:00~12:30

A thiazolium-based organic catalyst for the efficient utilization of atmospheric carbon dioxide

Hae-Jo Kim

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Thiamine pyrophosphate (ThPP) is a key coenzyme of pyruvate dehydrogenase, which transforms pyruvate into acetyl CoA to perform the Krebs cycle. Inspired by the ThPP, thiazolium and DMAP were utilized for carbon dioxide capture using epoxide and atmospheric CO₂ at mild temperature in 96% yield. The epoxide-to-cyclocarbonate transformation reaction was successfully even in the presence of a significant amount of moisture (100 mol% water).



Poster Presentation : **ORGN.P-155**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Triazole Calix[4]arene-Strapped Calix[4]pyrroles as Heteroditopic Ion Pair Receptors

Seung Hyeon Kim, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Calix[4]arene-calix[4]pyrrole hybrids connected via triazole units were synthesized and their binding properties for cations and anions as well as ion pairs were investigated in solution and in the solid state. It was revealed by ^1H NMR spectroscopic analyses that the ion pair receptors were able to bind specific ion pairs such as LiCl and CsCl with high affinity and selectivity over other alkaline metal chloride salts. It was also proved that the receptors formed complexes with LiCl and CsCl in two different binding modes. For instance, in the case of LiCl, the Li^+ cation was bound to the calix[4]arene moiety with the aid of the triazole groups with the Cl^- anion being bound to the calix[4]pyrrole unit. By contrast, the Cs^+ cation was bound to the bowl-shaped calix[4]pyrrole cavity formed as a result of the chloride binding to the calix[4]pyrrole unit.

Poster Presentation : **ORGN.P-156**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of a crown ether strapped-hexapyrrolic calix[4]pyrrole with amide linkage and its anion and ion pair recognition

Nam Jung Heo, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

The hexapyrrolic calix[4]pyrrole strapped with a crown ether via amide linkages was synthesized. ^1H NMR spectroscopic analyses revealed that the receptor was able to various anions such as the fluoride, the chloride, and the hydrogen phosphate anion with remarkably high affinity. This finding was ascribed to all of eight NHs playing a role in anion binding. It was also proved that the receptor bound the fluoride and the chloride anion in different binding modes. For example, in the case of the former anion, the pyrroles attached to the meso carbon of the calix[4]pyrrole framework take part in the fluoride binding via π -anion interaction. By contrast, the meso pyrroles participate in the binding of the chloride anion forming direct hydrogen bonds. The receptor was also found to bind LiCl and CsCl with high affinity. In this case, the lithium cation was complexed with the crown moiety while the chloride anion was hydrogen bonded to the NHs of the calix[4]pyrrole and the meso pyrroles as well as the amide NHs. On the contrary, in the case of CsCl, the cesium cation was presumed to be bound to the bowl shape of the calix[4]pyrrole cavity conformationally fixed as a result of the chloride binding.

Poster Presentation : **ORGN.P-157**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A tripodal heteroditopic receptor for anions, cations, and ion pairs

Juho Yang, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new tripodal ion receptor comprised of three pyridine groups and indole amide groups was synthesized. The receptor was found to bind cations with the pyridine constituents and anions with the indole and amide groups via hydrogen bonding interactions. In addition, the receptor proved capable of recognizing specific ion pairs, for example, LiCl. Upon the exposure of the receptor to anions, it displayed colorimetric responses to F⁻, HCO₃⁻, H₂PO₄⁻, and HP₂O₇³⁻ accompanying bathochromic shifts of its absorption band. These findings were taken as evidence for hydrogen bonding interactions between the receptor and such anions. On the other hand, the receptor was found to form complexes with certain cations such as Zn²⁺ and Li⁺. It was also revealed by ¹H NMR and UV spectroscopic analyses that the receptor was able to bind lithium chloride highly selectively over other alkali metal chloride salts.

Poster Presentation : **ORGN.P-158**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

New Macrocyclic Ion Pair Receptors Based on Indole Amides and Pyridines

Han-byeol Choi, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Heteroditopic macrocycles consisting of bis-indole amides and pyridines or polyethylene glycols were synthesized as ion pair receptors. The receptors were revealed to bind anions via hydrogen bonds between the NHs of the amide and indole subunits and cations using pyridines or the polyethylene glycol unit. For example, the receptors were found to recognize small anions such as the fluoride and the chloride anions with high selectivity. In this case, significant downfield shift of the proton signals of the amide and indole NHs was observed in ^1H NMR spectra, which was attributable to their formation of hydrogen bonds with the anions. On the other hand, they are capable of binding the lithium cations selectively over other alkaline metal cations. In addition, it was proved by UV/Vis spectroscopic analysis that the receptors formed the complexes with LiCl in solution as well as in the solid state.

Poster Presentation : **ORGN.P-159**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Phenanthroline-Strapped Calix[4]pyrroles as Highly Selective Receptors for the Bicarbonate Anion and the Lithium Chloride Ion Pair

Juhyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Calix[4]pyrroles strapped with phenanthroline via the ester and amide linkages have been synthesized. ¹H NMR spectroscopic analyses and single crystal X-ray diffraction analysis of the receptor with the ester linkages revealed that it was able to bind LiCl with high affinity and selectively and therefore to extract LiCl in solution as well as in the solid state. In this case, the lithium cation is bound to the nitrogen atoms of the phenanthroline and one of the oxygen atoms of the ester linkage while the chloride anion is hydrogen bonded to the NHs of the calix[4]pyrrole. On the other hand, the receptor having the amide linkages was found to bind the bicarbonate anion highly selectively over other anions including halides, the hydrogen phosphate, sulfate, and pyrophosphate. This high selectivity is attributable to the participation of the nitrogen atoms of the phenanthroline in the hydrogen bond with the bicarbonate anion.

Poster Presentation : **ORGN.P-160**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Small molecular cages as Anion Receptors with High Selectivity for the Fluoride Anion

Hye Jin Han, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Small molecular cages based on 1,3,5-trisubstituted benzene skeleton were synthesized as anion receptors for the selective recognition of the fluoride anion. The cages are comprised of three imines or amines as hydrogen bond acceptors and three pyrroles as hydrogen bond donors. ¹H NMR spectroscopic analysis showed that the cages were able to bind only the fluoride anions in the organic media even in the presence of various test anions such as halides, the hydrogen sulfate, the sulfate, the hydrogen phosphate, the pyrophosphate, the bicarbonate anions. This high selectivity for the fluoride anion is ascribable to the small size and the rigidity of the cavity formed by three imino-pyrrole groups. Further details on the synthesis and binding properties of the receptors will be presented.

Poster Presentation : **ORGN.P-161**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Melanosome targetable tyrosinase-selective ratiometric probe

Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Tyrosinase is an important biomarker of melanoma cancer because this enzyme overexpresses in melanoma cancer cells and it is considered as a promising target for cancer diagnosis and treatment. Tyrosinase is localized to the melanosomes in melanocytes. Here, we developed a morpholine-naphthalimide hybrid (**1**) as a ratiometric fluorescent probe that allows for a precise and quantitative analysis of tyrosinase activity. Probe **1** showed fluorescence changes at 460 and 560 nm for tyrosinase activity over other biologically relevant species, including metals, anions, and redox species. The kinetic parameters for the enzymatic reaction of probe **1** towards tyrosinase were determined by using Michaelis-Menten analysis. Also, inhibitory assay of tyrosinase activity was performed using **1** in the presence of kojic acid, a well-known tyrosinase inhibitor. As the concentration of kojic acid increases, the fluorescence ratio ($I_{560\text{ nm}}/I_{460\text{ nm}}$) was decreased. Now, confocal microscopy is in progress. We believe that probe **1** can provide a tyrosinase-dependent ratio fluorescent image and it is expected to be used for a real-time monitoring of tyrosinase activity in live melanoma cells.

Poster Presentation : **ORGN.P-162**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of coumarin-appended naphthalimide fluorescence probe for sensing and distinguishing hydrogen sulfide from other biothiols

Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Bitioliols, such as hydrogen sulfide (H₂S), cysteine, homocysteine, and glutathione, play important role in biological systems. The abnormal levels are directly associated with various human diseases. In this work, coumarin-appended naphthalimide **1** was developed as a multi-sensing fluorescence probe that can discriminate H₂S from other biothiols. Initially, probe **1** displayed a coumarin emission at 465 nm. However, in the presence of H₂S, the **1** exhibited a new emission at 550 nm was emerged, while the initial emission at 465 nm was constant. By measuring the fluorescence intensities at 465 and 550 nm we could obtain a ratiometric fluorescence signal change towards H₂S concentration. On the other hands, in the case of cysteine, homocysteine, and glutathione, probe **1** showed fluorescence enhancements at 500 nm. Therefore, we could distinguish the H₂S from other biothiols by monitoring the fluorescence intensity (FI) at 465 nm and FI ratio ($I_{630\text{ nm}}/I_{465\text{ nm}}$). Moreover, the limits of detection for GSH and H₂S were calculated to be 6.6 μM and 1.2 μM, respectively. Furthermore, the sensing mechanisms of probe **1** for H₂S and other thiols were thoroughly investigated by using HPLC and ESI-Mass analyses.

Poster Presentation : **ORGN.P-163**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

An efficient resorufin-based fluorescent Off-On probe for selective detection of nitroreductase in bacteria

Jung Won Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Bacteria are living things that composed only one cell. There are various types of bacteria in human's body that function differently, including digestion, destruction of cells that cause diseases, and production of vitamins. However, some bacteria can cause harm to human's body resulting infections. So, it is very important to detect bacteria efficiently. Nitroreductase (NTR) is a well-known enzyme that exists in bacteria, NTR is often used as a biomarker for detecting bacteria. We presented resorufin-based probes (**1** and **2**) as a fluorescent Off-On probe for detection of nitroreductase (NTR) activity. Towards NTR activity, these probes gave a fluorescence turn-on at 586 nm with a visual color change from colorless to pink. The sensing ability, mechanism, and enzyme kinetics of the probes for NTR were thoroughly investigated by using absorption, fluorescence, and ESI-Mass spectroscopic analyses. Enzyme efficiencies of the probes were evaluated as 0.260 and 4.368 $\mu\text{M}^{-1}\text{s}^{-1}$, respectively, revealing a high sensitivity to NTR activity compared to other previously reported probes. Particularly, probe **1** exhibited an excellent detection ability for NTR activity with a no background signal and a high selectivity in comparison with probe **2**. Thus, we are believing that probe **1** as an efficient fluorescent Off-On probe for NTR activity with a fast response, good selectivity and sensitivity, as well as a high signal to noise. We are now going on more experiments using probe **1** for monitoring the change of NTR activity in a variety of bacteria.



Poster Presentation : **ORGN.P-164**

Organic Chemistry

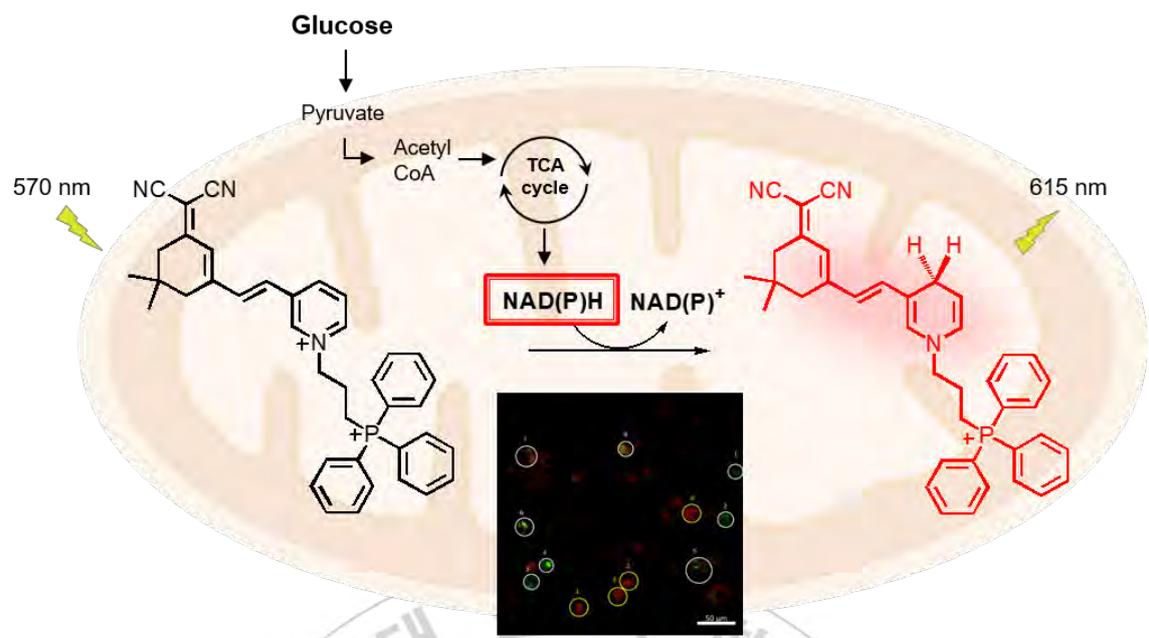
Exhibition Hall 2, THU 11:00~12:30

Mitochondrial NAD(P)H targetable red-emitting fluorescent probe and its application in real-time monitoring of live cells

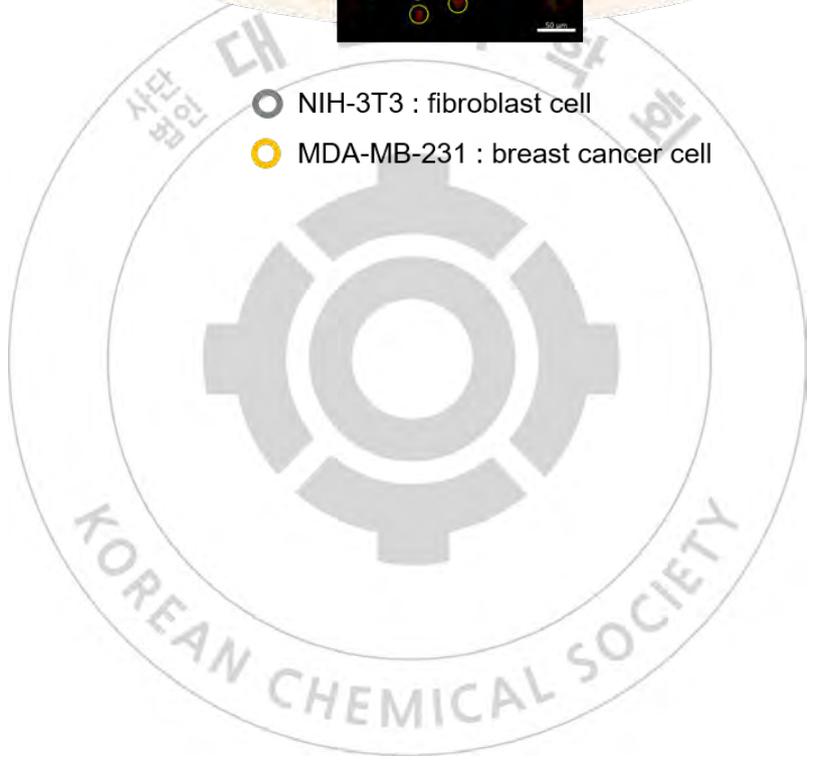
Jin Hui Joo, Sun Young Park, Min Hee Lee*

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. Probe **1** is none-fluorescent, however, upon reacting with NAD(P)H a significant fluorescence increase was monitored in both solution and living human breast cancer cells (MDA-MB-231 cell). Furthermore, probe **1** can be used to differentiate between cancer (MDA-MB-231) and normal cells (NIH-3T3) based on mapping mitochondrial NAD(P)H-dependent fluorescence intensity. Probe **1** will be useful for various applications, ranging from elucidation of biological pathways to pathological diagnosis.



- NIH-3T3 : fibroblast cell
- MDA-MB-231 : breast cancer cell



Poster Presentation : **ORGN.P-165**

Organic Chemistry

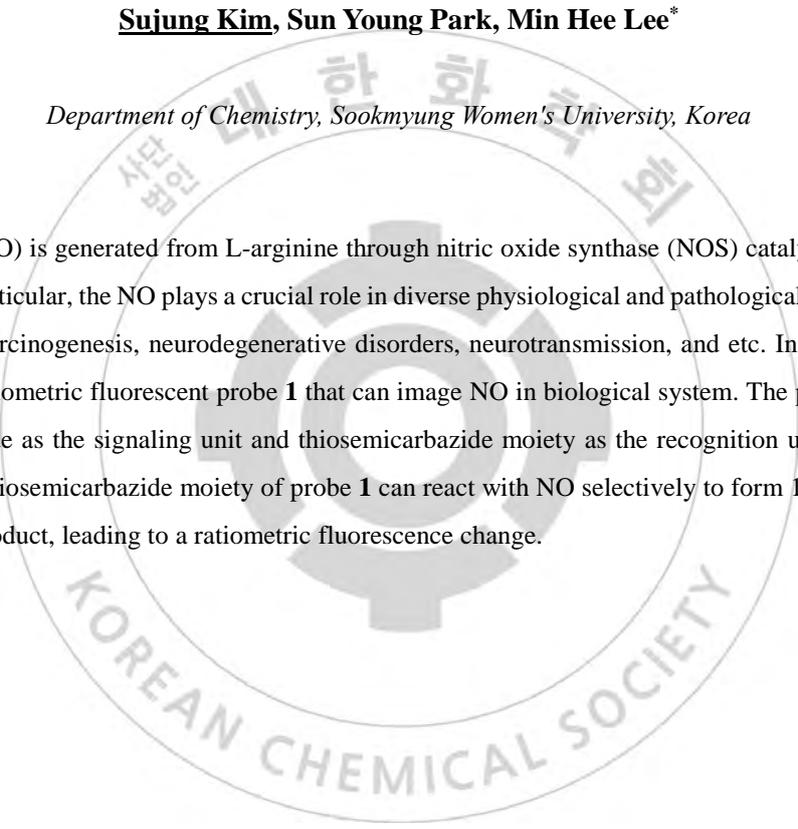
Exhibition Hall 2, THU 11:00~12:30

A fluorescent naphthalimide bearing thiosemicarbazide as a ratiometric fluorescent probe for the detection of nitric oxide

Sujung Kim, Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Nitric oxide (NO) is generated from L-arginine through nitric oxide synthase (NOS) catalyzed reaction in live cells. In particular, the NO plays a crucial role in diverse physiological and pathological processes, e.g., vasodilation, carcinogenesis, neurodegenerative disorders, neurotransmission, and etc. In this regard, we developed a ratiometric fluorescent probe **1** that can image NO in biological system. The probe **1** consists of naphthalimide as the signaling unit and thiosemicarbazide moiety as the recognition unit for NO. We think that the thiosemicarbazide moiety of probe **1** can react with NO selectively to form 1,3,4-oxadiazole heterocyclic product, leading to a ratiometric fluorescence change.



Poster Presentation : **ORGN.P-166**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Acrylamide-coumarin-benzaldehyde as a turn-on fluorescent probe providing an enhanced water solubility for detection of cysteine and homocysteine

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Department of chemistry, Sookmyung Women's University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

We presented a turn-on fluorescent probe (**1**) for Cys/Hcy based on Michael addition reaction with Cys/Hcy. Probe **1** is composed of benzaldehyde-conjugated coumarin as a water-soluble fluorophore and acrylamide group as a Michael addition site for Cys/Hcy as well as fluorescence quencher. Initially, probe **1** is almost non-fluorescent due to PET process from the acrylamide group. However, in the presence of Cys/Hcy, **1** showed strong blue fluorescence at 420 nm owing to a PET inhibition resulted from Michael addition reaction of acrylamide group of **1** with Cys/Hcy. The detection mechanism of **1** for Cys/Hcy was identified by ESI-MS and ¹H NMR analyses. Additionally, the fluorescence enhancement of **1** was selectively monitored to Cys/Hcy over other biologically potential interferants including GSH, H₂S, RONS, anions, and metal ions. Besides, **1** can give fluorescence turn-on for Cys/Hcy in the wide pH range of 2-11 and the limit of detections (LOD) for Cys and Hcy turned out to be 17.25 and 8.69 μM. As a result, we could suggest that fluorescent probe **1** would be widely applied to monitoring Cys and Hcy present in most physiological conditions.

Poster Presentation : **ORGN.P-167**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Series of Guanidine Conjugates with NSAID

Ju Mi Lee, Jeong Tae Lee*

Department of Chemistry and Institute of Applied Chemistry, Hallym University, Korea, Hallym University, Korea

The guanidine derivative (9,13*b*-dihydro-1*H*-dibenzo[*c,f*]imidazo[1,5-*a*]azepin -3-amine hydrochloride) (**1**) is a fat cell stabilizer commonly used in eye inflammation caused by an allergic reaction. It is an optional H1 receptor antagonist which does not cross the blood brain barrier. Herein, a series of guanidine containing nonsteroidal anti-inflammatory drugs (NSAIDs) conjugates were synthesized based on coupling of different NSAIDs such as aspirin and salicylic acid with **1**. Additionally, synthetic approach to other conjugates containing γ -aminobutyric acid (GABA) (neurotransmitter) and gabapentin (anticonvulsant agent) moieties as linkers as well as their biological evaluation are also in progress.

Poster Presentation : **ORGN.P-168**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Syntheses and Biological Activities of Resveratrol Analogs with Nitrogen

Lee Seul Park, Jeong Tae Lee*

Department of Chemistry and Institute of Applied Chemistry, Hallym University, Korea, Hallym University, Korea

Nitrogen-based heterocycles are important motifs in drug design and engineering of pharmaceuticals. A simple glance at FDA databases reveals that nearly 60% of unique small-molecule drugs containing a nitrogen heterocycle. Resveratrol (3,5,4'-*trans*-trihydroxystilbene) is a natural product known to exhibit strong antioxidant activity. To enhance its antioxidant efficacy, we have synthesized nitrogen-based heterocycles (quinoline, isoquinoline, quinoxaline, and quinazoline) containing resveratrol analogs using Wittig-Horner and metal-catalyzed reactions as key synthetic steps. Later, their antioxidant activity was measured by the ABTS assay and IC₅₀ values of these compounds were also calculated.

Poster Presentation : **ORGN.P-169**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Bioactive Homoisflavonoids: Synthesis and Antiinflammatory Activity

Damodar Kongara, Jong-Gab Jun*, Jeong Tae Lee*

Department of Chemistry and Institute of Applied Chemistry, Hallym University, Korea, Hallym University, Korea

This study describes the first synthesis of natural homoisflavonoids, (\pm)-portulacanonones A-C (**4**, **8** and **9**), portulacanone D (**6**) isolated from *Portulaca oleracea* L (POL) and their derivatives (**3**, **5** and **7**) along with the synthesis of known derivatives (**1** and **2**) and also evaluation of their *in vitro* inhibitory effect against nitric oxide (NO) production in LPS-induced RAW-264.7 macrophages. All the compounds exhibited a concentration-dependent inhibitory effect and had no significant cytotoxicity to the macrophages at their effective concentration for the inhibition of NO production. Among them, compounds **3** (97.2% at 10 μ M; IC_{50} = 1.26 μ M) followed by **6** (92.5% at 10 μ M; IC_{50} = 2.09 μ M), **1** (91.4% at 10 μ M; IC_{50} = 1.75 μ M) and **7** (83.0% at 10 μ M; IC_{50} = 2.91 μ M) exhibited pronounced inhibition from the series. The obtained results were further correlated with the suppressed expression of iNOS induced by LPS. On the whole, compound **3** is expected to serve as a lead structure that merits further investigation for a NO production-targeted anti-inflammatory drug development and also could evidence the practicality of POL as a folklore medicinal plant in the treatment of inflammatory diseases where NO is involved.

Poster Presentation : **ORGN.P-170**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Visible-Light Photocatalyzed Deoxygenation of N-Heterocyclic N-Oxides

Kyu Dong Kim, Jun Hee Lee*

Department of Advanced Materials Chemistry, Dongguk University, Korea

Deoxygenation reactions that furnish N-heterocycles in a chemoselective manner represent a fundamental transformation in organic synthesis. Despite the recent invention of several successful implementations of these reactions, such approaches commonly require the use of oxophilic reagents or intermediates at high temperatures. In this context, the development of a new method for the room temperature deoxygenation of N-heteroaromatic N-oxides would be useful if the otherwise labile functional groups are compatible with the reaction conditions. To this end, as part of our ongoing program to develop new transformations via visible-light-induced photoredox catalysis,¹ we recently developed a scalable and operationally simple method that allows for the chemoselective room temperature deoxygenation of a wide range of N-heterocyclic N-oxides using only commercially available reagents.² Notably, a highly chemoselective removal of the oxygen atom in a quinoline N-oxide was accomplished successfully for the first time through the judicious choice of the photocatalyst even in the presence of a pyridine N-oxide in the same molecule. Another notable feature of this visible-light-induced photocatalytic protocol is the unprecedented oxidation of hydrazine hydrate using heterocyclic N-oxides as a mild oxidant for the convenient in situ generation of diimide under ambient conditions. Further details of this useful protocol will be discussed in the presentation.

Poster Presentation : **ORGN.P-171**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Metal-free Formylation of Amines

Seul Chan Lee, Hye-Young Jang^{1,*}

Department of Energy System, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

To develop sustainable and environmentally-friendly technologies, utilization of greenhouse gases like carbon monoxide(CO), carbon dioxide(CO₂) and methane(CH₄) has been studied widely. A variety of processes using these gases have been investigated and commercialized, in particular, carbonylation using carbon monoxide(CO) has also been employed in commercial processes for producing chemical products. For example, Fischer-Tropsch process, acetic acid synthesis, and hydroformylation are known. Most of carbonylation processes require expensive transition metal catalysts like iridium, rhodium, cobalt, iron and nickel because CO is not reactive toward organic compounds. In this study, we focused on the formylation of amines using CO in the absence of metal catalysts. Detailed reaction conditions and results are discussed.

Poster Presentation : **ORGN.P-172**

Organic Chemistry

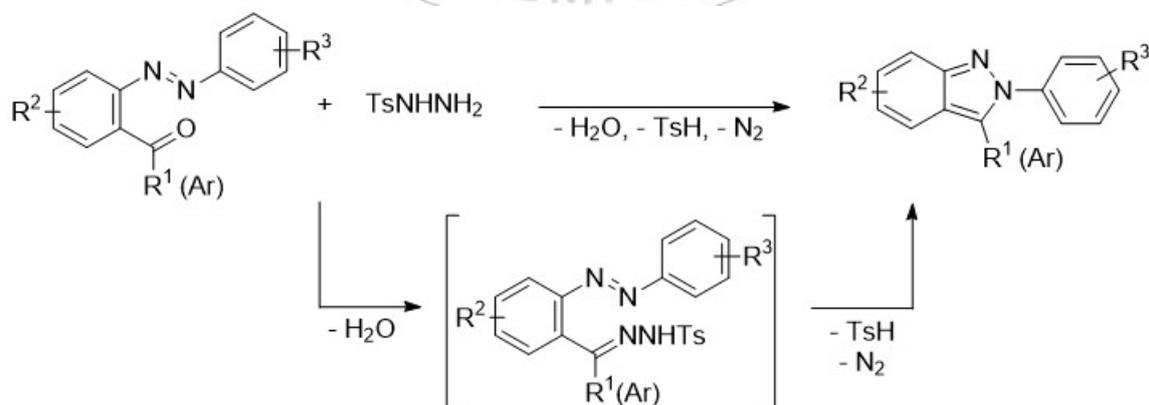
Exhibition Hall 2, THU 11:00~12:30

Tosyl Hydrazine-Promoted Tandem Condensation and Cyclization of Acyl Azobenzenes Enabling Access to 2H-Indazoles under Metal-Free Aerobic Conditions

Seungcheol Lee, Sang Hoon Han, Younghyeon Baek, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

We envisioned that the treatment of 2-acyl azobenzenes with tosyl hydrazine would produce the corresponding tosyl hydrazones along with the release of water, and then, the hydrazones would be easily transformed to 2-aryl-2H-indazoles having 3-alkyl- or 3-aryl groups through intramolecular cyclization with concomitant release of molecular nitrogen and sulfinic acid under metal-free conditions. Herein, we describe an efficient synthetic method for 2-aryl-2H-indazoles having alkyl- or aryl groups at the 3-position through intramolecular cyclization of tosyl hydrazone having an azobenzene moiety, which is generated in situ from the condensation of 2-acyl azobenzene with tosyl hydrazine together with the release of water, molecular nitrogen, and sulfinic acid under metal-free aerobic conditions. All of the examples produced the corresponding 2H-indazoles in quantitative yields. The present reaction was determined to have a wide substrate scope and good functional group tolerance.



Poster Presentation : **ORGN.P-173**

Organic Chemistry

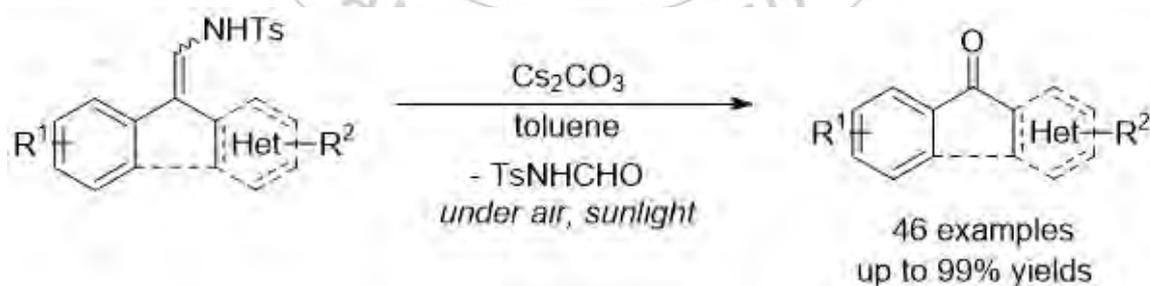
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Diaryl Ketones through Oxidative Cleavage of the C–C Double Bonds in *N*-Sulfonyl Enamides

Seungcheol Lee, Gi Hoon Ko, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

An oxidative cleavage of a C–C double bond is developed from the 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 a 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 the Cu-catalyzed [3+2]-cycloaddition, Rh-catalyzed alkoxyarylation, photooxygenation, and ring-opening reaction in one-pot. Because the 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-174**

Organic Chemistry

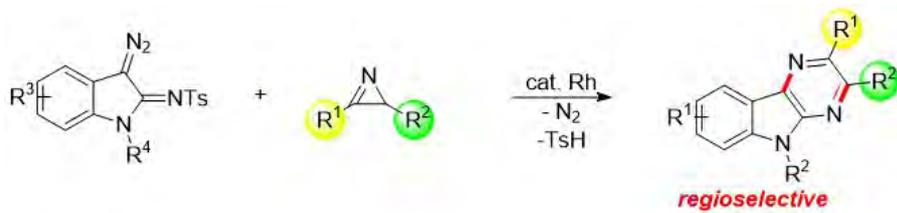
Exhibition Hall 2, THU 11:00~12:30

Regioselective Synthesis of Indolopyrazine via a Sequential Rh-Catalyzed Formal [3 + 3] Cycloaddition and Aromatization Reaction of Diazoindolinimines with Azirines

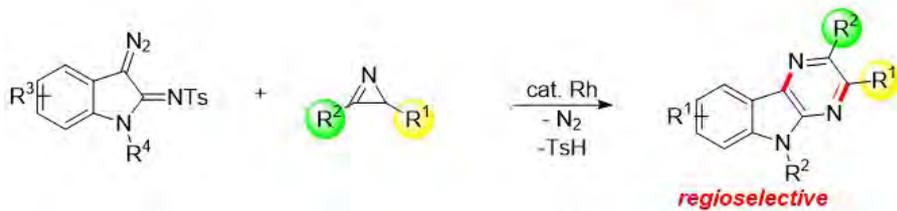
Hyung Jin Seo, Gi Uk Han, Younghyeon Baek, Phil Ho Lee*

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-175**

Organic Chemistry

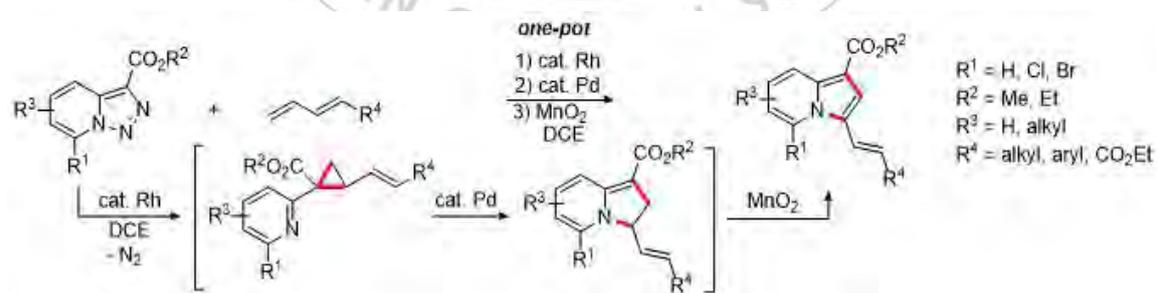
Exhibition Hall 2, THU 11:00~12:30

One-Pot Synthesis of Indolizines Derivatives through Sequential Rh-Catalyzed [2 + 1]-Cyclopropanation, Pd-Catalyzed Ring Expansion, and Oxidation Reactions from Pyridotriazoles and 1,3-Dienes

Hyung Jin Seo, Chanyoung Maeng, Kyungsup Lee, 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-176**

Organic Chemistry

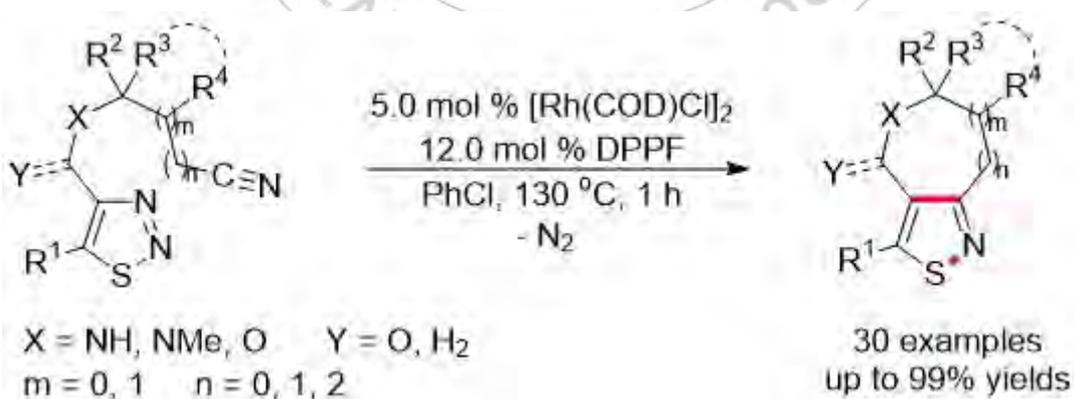
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Bicyclic Isothiazoles *via* Intramolecular Rh-Catalyzed Transannulation of Cyanothiadiazoles

Juyoung Heo, Gi Uk Han, Kyungsup Lee, 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-177**

Organic Chemistry

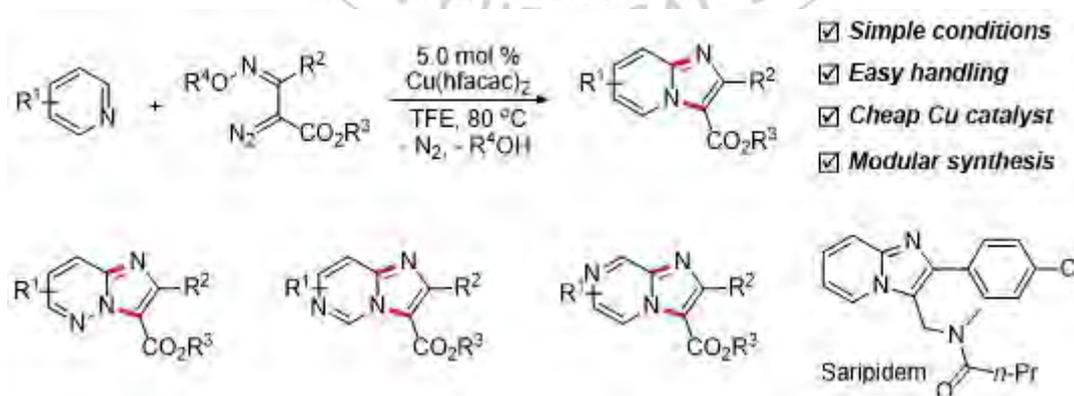
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Imidazopyridines *via* a Copper-Catalyzed, Formal Aza-[3 + 2] Cycloaddition Reaction of Pyridine Derivatives with α -Diazo Oxime Ethers

Juyoung Heo, Gi Hoon Ko, Gi Uk Han, 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.



Poster Presentation : **ORGN.P-178**

Organic Chemistry

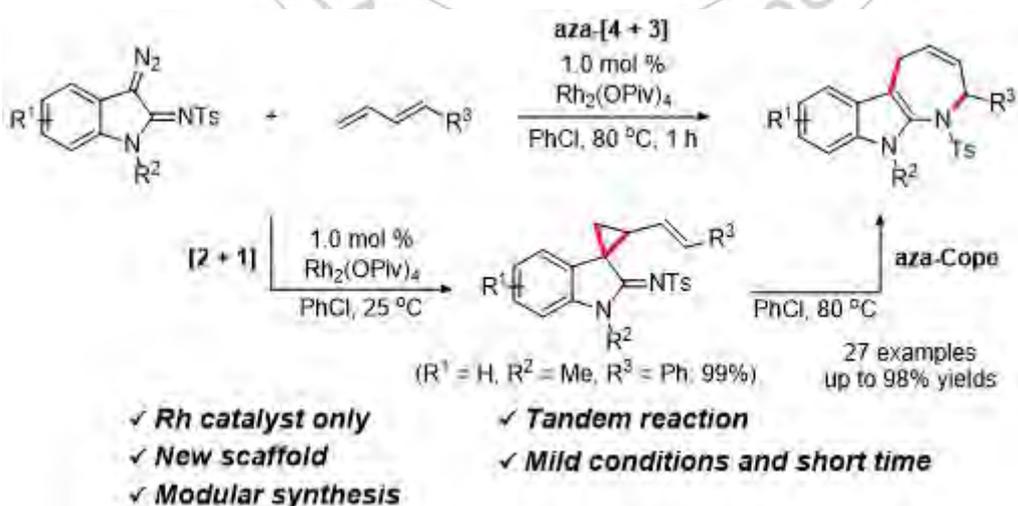
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Azepinoindoles *via* Rhodium-Catalyzed Formal Aza-[4 + 3] Cycloaddition Reaction of 3-Diazoindolin-2-imines with 1,3-Dienes in One-Pot

Sejin Jang, Chanyoung Maeng, Sang Hoon Han, 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-179**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Pyrazinoindole-Based Lewis-Acid/Base Assembly: Intriguing Intramolecular Charge-Transfer Switching through the Dual-Sensing of Fluoride and Acid

Sejin Jang, Chanyoung Maeng, Gi Hoon Ko, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Pyrazinoindole-based Lewis-acid/base assemblies are prepared through the use of regioselective formal [3 + 3] cycloaddition reactions and their intriguing photophysical properties are described. The assemblies exhibit strong emissions in THF solution, which are attributed to through-space intramolecular charge-transfer (ICT) transitions between the branched Lewisacid/ base moieties. Furthermore, these show ratiometrically color-change responses in PL titration experiments, which give rise to new colors through turn-on emissions ascribable to ICT transitions that alternate between the pyrazinoindole units and each triarylboron or amino moiety, a consequence of the binding of the fluoride or acid. Pieces of filter paper covered by these assemblies demonstrated exhibited blue-shifted color changes when immersed in aqueous acidic solutions, suggesting that these are promising candidate indicators that detect acid through emissive color. Computational data for these assemblies and their corresponding adducts verify the existence of ICT transitions that alternate through fluoride or acid binding.

Poster Presentation : **ORGN.P-180**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Transfer Hydrogenation of Carbonates in Glycerol

Kihyuk Sung, Yeon Joo Cheong¹, Hye-Young Jang^{2,*}

Department of Energy System Research, Ajou University, Korea

¹*Department of Energy System, Ajou University, Korea*

²*Department of Chemistry, Ajou University, Korea*

Glycerol has environmental advantages such as nontoxicity and biodegradability, and economic advantages supplied from biodiesel industries. Therefore, various chemical conversions using glycerol have been developed. Transfer hydrogenation is a reaction which transfers hydrogen atoms to organic compounds in the absence of H₂ gas. It is difficult and dangerous to handle H₂ gas as the hydrogen source, so we investigated other hydrogen sources instead of H₂ gas. Due to the many advantages of glycerol, glycerol is used as a hydrogen source to reduce organic carbonates. In addition to the hydrogen source, the economic feasibility of this reaction can be increased via transformation of glycerol to lactic acid after transfer hydrogenation. In this presentation, we present detailed conditions and reaction results of transfer hydrogenation of carbonates.

Poster Presentation : **ORGN.P-181**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Activity Evaluation of Materials having excellent Liver cancer prevention and Anti-cancer activity

Songmi Bae, Ju Hyun Song, Eon Jin Lee, Do hun Lee, Jong Hyun Cho¹, Dai Il Jung*

Department of Chemistry, Dong-A University, Korea

¹Department of Medicinal, Dong-A University, Korea

NAFLD is non-alcoholic fats, which is a type of fatty liver that occurs when fat builds up in the liver for reasons other than excessive alcohol use. Up to 80 percent of obese people have this disease. It is the most common liver disorder in developed countries. If found early on and treated, the results can be good, but it can develop into non-alcoholic steatohepatitis (NASH) for various reasons, leading to liver sclerosis and liver cancer. By Niche chemistry(esterification and acid condensation) we researched development of fresh and original medicines. Esters are formed from bioactive carboxylic acids and bioactive alcohols. Acid anhydrides can be obtained from condensation reaction known as a dehydration reaction. The substances we synthesized, ester and acid anhydride, are separated by a cation and anion with physiological activity, or separated by the original active substance, to represent their physiological activity, even before being passed to the blood when administered to the body. By applying this reaction process, we developed materials that have excellent liver cancer prevention and anti-cancer activity as well as new diet effects with low side effects and adverse reactions.

Poster Presentation : **ORGN.P-182**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesized Curcumin Derivatives Target to β -amyloid Plaque by Optical Imaging of the Eye.

Suah Yoo, Haebin Kim, Kyo-Chul Lee^{1,*}, Dong Wook Kim^{2,*}

Inha University, Korea

¹*Korea Institute of Radiological & Medical Science, Korea*

²*Department of Chemistry, Inha University, Korea*

It has been demonstrated that the brain of Alzheimer's disease (AD) patient is more stained by staining solutions than healthy brain because of an interaction between a staining solution and β -amyloid ($A\beta$) plaques. The deposition of β -amyloid ($A\beta$) plaques in the brain is the most significant target of molecular imaging due to a major pathological property of Alzheimer's disease (AD). As flat structures of a compound fit into hydrophobic binding channels of $A\beta$ plaques easily, the rigid conjugation planarity compounds have been used to detect the $A\beta$ plaques. A visualization of cerebral $A\beta$ plaques is considered to be the most feasible way to diagnose AD. However, almost common probes for AD showed relatively high nonspecific white matter uptake probably due to myelin uptake. This is an obstacle to demarcate the borders of the gray matter, where the $A\beta$ plaques binding signals. Recently, it has been suggested that the Alzheimer's peptide, $A\beta$, accumulates in the eye. In this study, PEGylated curcumin derivatives were synthesized for binding to $A\beta$ plaques with high photoluminescence and enhanced blood circulation. Our synthesized PEGylated curcumin derivatives exhibit red region fluorescences which are appropriate biological $A\beta$ plaques of optical imaging for AD diagnosis in the eye.

Poster Presentation : **ORGN.P-183**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Helical Columnar Assemblies of Discotic liquid crystals based 1,2,3-triazole depending on chain structure

Youngmin Lee, Byoung-Ki Cho*

Department of Chemistry, Dankook University, Korea

1,2,3-Triazole that can be easily synthesized by copper-catalyzed click reaction, is an asymmetric aromatic group, and thereby would be a useful structural motif in the design of functional liquid crystals (LCs). Recently, we synthesized two types of 1,2,3-triazole based C_3 -symmetric LCs through the click reaction of 1,3,5-triethynylbenzene and 4-azido-1,2-bis(alkoxy)benzene. Two LCs consist of different aliphatic chains, which are linear and chiral chains, respectively. The LCs were characterized using differential scanning calorimetry (DSC), wide-angle X-ray scattering (WAXS), grazing-incidence wide-angle X-ray Scattering (GIWAXS) and dielectric relaxation spectroscopy (DRS). The LC with chiral chains showed a melting transition at 105.8 °C, while the LC with linear chains shows no melting transition. From the GIWAXS analyses the LCs exhibited different helical columnar structures at room temperature. This structural difference can be explained by the packing variation which might be affected by the chain structure. All the details will be addressed in poster presentation.

Poster Presentation : **ORGN.P-184**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and modification of hetero-functionalized internal alkynes

Seo Young Jeong, Sung You Hong*

Ulsan National Institute of Science and Technology, Korea

We described here a synthesis of internal alkynes (cyano group and thio group). Contents include: (1) we synthesized cyanoalkynes by the procedure of Sonogashira coupling of iodobenzene to propargyl alcohol and then into nitriles with ammonium acetate, iodobenzene diacetate and TEMPO. (2) we synthesized thioalkynes into an one-pot from terminal alkyne via the nucleophilic substitution of lithium alkynyl thiolate to diverse halides with n-BuLi and sulfur.



Poster Presentation : **ORGN.P-185**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Regioselective synthetic strategy of β -hydroxy sulfones

Hyowon Park, Hye-Young Jang^{1,*}

Department of Energy Systems Research, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

β -Hydroxy sulfones are synthesized by transition-metal catalyzed reactions, oxidant-mediated hydroxyl sulfonylation of alkenes, and ring opening reaction of epoxides with sulfinate salts. The previous reports show excellent yields, but they have environmental problems using toxic reagents and chemical issues related to regioselectivity issues. Moreover, commonly used sulfinate salts are relatively unstable and commercially limited. Therefore, it is important to develop an eco-friendly synthetic method for β -hydroxy sulfones in a regioselective manner. We investigated a regioselective β -hydroxy sulfones synthetic method using thiosulfonates as sulfonylating reagents, which are easily accessible by copper-catalyzed coupling of thiols. In this presentation, we will discuss detailed optimizations, substrate scopes, and the mechanism.

Poster Presentation : **ORGN.P-186**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Visible-light-promoted synthesis of biaryl compounds

Boseok Hong, Anna Lee*

Department of Chemistry, Myongji University, Korea

Biarenes are a commonly found moiety in various natural products, bioactive compounds, and synthetic intermediates. Because of their structural importance, development of novel and more efficient synthetic methods have received significant attention from the organic communities over decades. The most common strategy to access the biaryl scaffold is the well-known transition metal catalyzed aryl-aryl coupling reactions such as Suzuki, Negishi, Ullmann, Stille, and Kumada coupling etc. These synthetic methods have provided powerful tools for synthesizing biaryl compounds, but they still have limitations like using toxic, expensive reagents and/or reacting under harsh conditions. Therefore, the development of more mild and efficient strategies would be greatly valuable for the construction of Aryl-Aryl bonds. Here in, we report visible-light-mediated aryl-aryl coupling reaction that does not need any metal catalysts or photosensitizer. This novel and environmentally benign method provides an alternative route to established synthetic approaches to afford the desired products from easily available substrates in high yields.

Poster Presentation : **ORGN.P-187**

Organic Chemistry

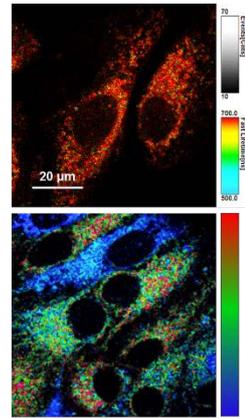
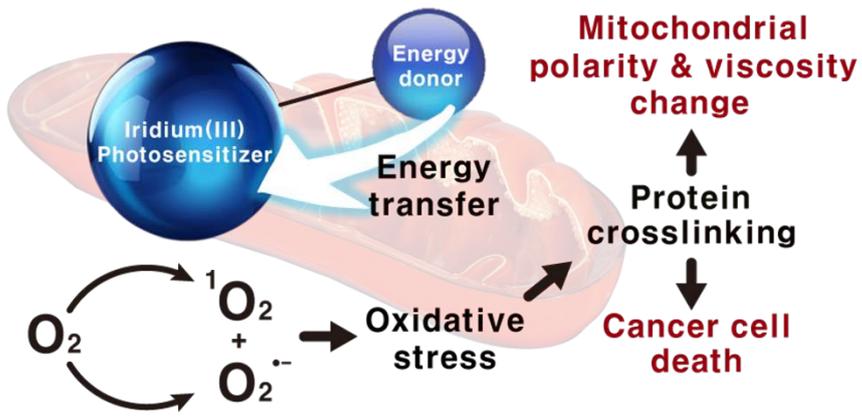
Exhibition Hall 2, THU 11:00~12:30

Intramolecular Energy Transfer based Ir(III) Photosensitizer for Inducing Mitochondrial Oxidative Stress and Monitoring Response

Chaiheon Lee, Jung Seung Nam, Tae-Hyuk Kwon*

Chemistry, Ulsan National Institute of Science and Technology, Korea

Mitochondria, one of cellular organelles, are involved in ATP production, maintenance of calcium homeostasis, cell growth, differentiation, and apoptosis. Mitochondrial oxidative stress induced by reactive oxygen species (ROS) damage physiological characteristics, and cause apoptosis as the oxidative stress of the cell exceeds the threshold. Therefore, inducing mitochondrial oxidative stress is efficient target for proceeding photodynamic therapy (PDT). Recently, iridium(III) complexes have attracted attention as photosensitizer for photodynamic therapy (PDT) because of their characteristics including high ROS generation efficiency, high stability in physiological condition. However, they have a limitation of low absorption coefficient in the visible region, which let high-energy irradiation ($>35 \text{ J/cm}^2$) necessary for iridium(III) based PDT. Herein, we report mitochondria-localized Iridium(III) photosensitizer, Ir-OA, incorporating acedan dye as energy donor. The acedan dye has strong absorbance and fluorescence which is well matched to the absorbance of iridium complexes. As the Ir-OA is irradiated, the absorbed energy by acedan donor is transferred to the iridium(III) with high efficiency ($>98\%$). As a result, the enhanced amount of triplet exciton of Ir-OA improved ROS generation, which cause effective cell death with ultra-low energy irradiation (



Poster Presentation : **ORGN.P-188**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

s-Triazine Based Oxidized Carbon Nitride : Directly ^{64}Cu -Chelatable for PET Imaging

Chul Hee Kim, Chan Ho Park, Kyo-Chul Lee^{1,*}, Dong Wook Kim^{2,*}

Inha University, Korea

¹*Korea Institute of Radiological & Medical Science, Korea*

²*Department of Chemistry, Inha University, Korea*

Radio-labelled nanoparticles have been expected as one of the powerful imaging probe for diagnosing various diseases in modern positron emission tomography (PET). The conventional method to label radioactive metal ion to the nanoparticle is using chelators from its surface. However, functionalization of these chelators to nanoparticles was often strictly limited due to the properties of nanoparticles like absent of functional groups, sensitivity to harsh reaction conditions and low-functionalization yield. Here we suggest directly ^{64}Cu -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 ^{64}Cu -chelatable nature and targeting ability toward tumor by experiment on animals.

Poster Presentation : **ORGN.P-189**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Study of Charge Transfer Dynamics in Dyes with Vibrational Spectroscopy and Computational Method

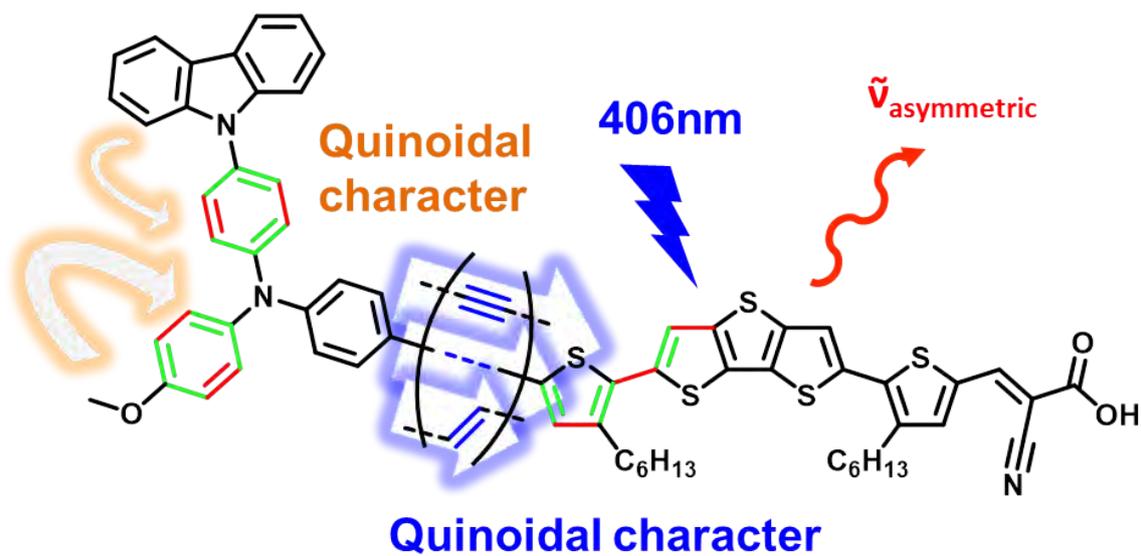
Wanghyo Kim, Joseph Mapley^{1,*}, Keith Gordon^{1,*}, Tae-Hyuk Kwon^{2,*}

Chemistry, Ulsan National Institute of Science and Technology, Korea

¹*Chemistry, University of Otago, New Zealand*

²*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

Enhancing the efficiency of charge transfer in dye is one of the most important issues for developing highly efficient dye-sensitized solar cells. Herein, we use resonance Raman spectroscopy (RRS) to study the effect of bond type and electron-donating groups on intramolecular charge transfer (ICT) of dithieno[3,2-b:2',3'-d]thiophene based dyes. All the dyes have the enhanced Raman shifts for the donor moieties at the identical positions, supporting the donor is involved in ICT. The density functional theory (DFT) calculation elucidates that the triple bond and the electron-donating groups enhance the ICT of donor for the first and third electronic transitions. This is consistently supported by RRS which shows enhancement thiophene bands for all transitions as well as selective enhancement of donor and triple bond bands when the third electronic transition is probed. This suggests that ICT is enhanced by quinoidal character mixed in π -conjugation bridge. This study shows the potential of TD-DFT and RRS for studying the relation of the structure and the enhancement of ICT in organic dyes.



Poster Presentation : **ORGN.P-190**
Organic Chemistry
Exhibition Hall 2, THU 11:00~12:30

Simple and Practical Synthetic Procedure for Amides from Trichloroethyl Esters Using 1,5-diazabicyclo[4.3.0]non-5-ene

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Amides are one of the most common functional groups in organic chemistry. Besides amide units play an important role in living systems such as amino acid linkage sites in peptide and protein. Thus, many synthetic methods of amides have been developed for many years. One of widely used methods is coupling reactions between a carboxylic acid and an amine. Carboxylic acids are commonly used in their protected form as esters during many chemical syntheses. The 2,2,2-trichloroethyl group is known to be an efficient carboxylic acid protecting group. This study describes direct synthesis of amides from 2,2,2-trichloroethyl esters. Several organic reagents and solvents were investigated for the preparation of amides from 2,2,2-trichloroethyl esters, and 1,5-diazabicyclo[4.3.0]non-5-ene and MeCN solvent system could yield desired amides. This procedure showed that a variety of target amide structures were synthesized in high yield successfully.

Poster Presentation : **ORGN.P-191**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Efficient Direct Synthesis Thioesters from Aldehyde Using Dibromoisocyanuric Acid

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Thioester is one of the commonly found chemical moieties in organic chemistry. In additions, thioester units have been found in a variety of natural products and bioactive molecules, and play crucial role of many pharmaceuticals. Coupling reactions of carboxylic acids and thiols is one of common preparation of thioester. Besides, recently aldehydes can be used to produce several thioester structures. Oxidative thioesterification procedure of aldehyde usually performed in harsh reaction such as high temperature. Thus, development of more mild reaction methods is still important to synthesis of thioester from aldehydes. In this study, novel direct conversion of aldehydes into thioesters under mild condition was presented. In the protocol, reaction of aldehyde with dibromoisocyanuric acid could produce acyrbromide intermediates at room temperature, and then treatment with thiols could produce the target thioesters with high yield.

Poster Presentation : **ORGN.P-192**

Organic Chemistry

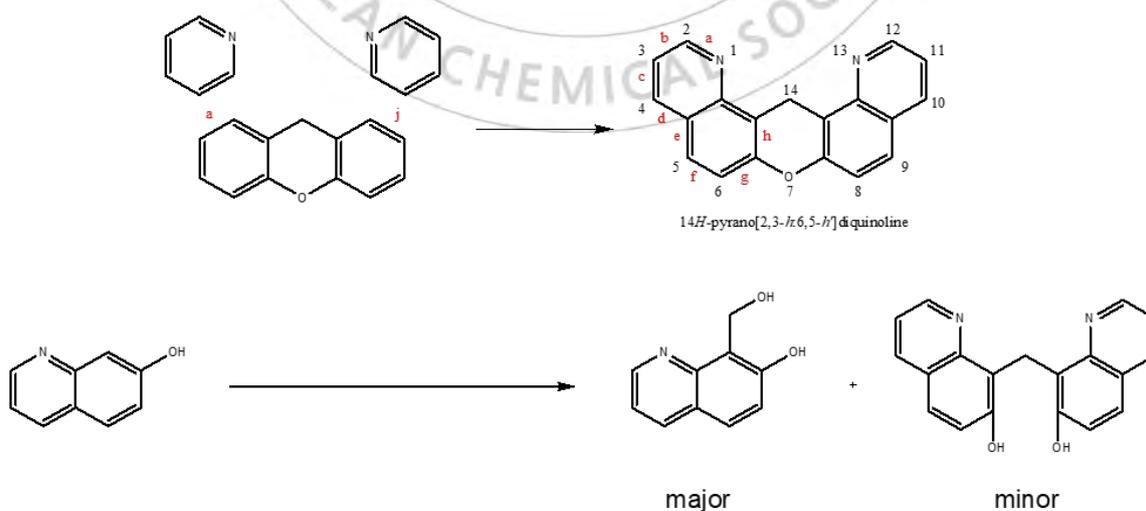
Exhibition Hall 2, THU 11:00~12:30

Serendipitous Synthesis of 14*H*-Pyrano[2,3-*h*:6,5-*h'*]diquinoline

Youngchan Bang, Bongjin Moon*

Department of Chemistry, Sogang University, Korea

Xanthene is an important structural motif in designing dyes and biologically active compounds due to its unique optoelectronic properties and planar structure with a heteroatom. Although numeral methods and tremendous number of xanthene derivatives are known, not many xanthene derivatives with heterocycles on *a*- and *j*- sides have been reported. During our recent study on the synthesis of quinoline derivatives, we serendipitously obtained a dimeric bisquinoline product as a minor component. The minor product could be derivatized into a xanthene derivative with two pyridine rings on *a*- and *j*- sides (14*H*-pyrano[2,3-*h*:6,5-*h'*]diquinoline) by simple treatment with sulphuric acid at high temperature (130 °C, 2 days). The structure was elucidated by X-ray crystallography. It was surprising that the carbon at 14-position was oxidized to alcohol under the reaction conditions. It was found that the hydroxyl group could be gradually exchanged with an alcohol without any catalyst.



Poster Presentation : **ORGN.P-193**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Practical and Simple Iron-mediated Transformation of Alcohol using 2-Diphenylmethoxypyridine into Diphenylmethyl Ethers

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Protection and deprotection are common methodologies used in organic reactions. Diphenylmethyl (DPM) ether, one of protection groups, has been widely employed for the protection of alcohol. In additions, many bioactive compounds such as enzyme inhibitors, antibacterial agents, and anticancer agents contain diphenylmethyl ether structures. Thus, several synthetic methods of diphenylmethyl ethers from alcohols have been studied. In this study, novel efficient transformation of alcohols using 2-diphenylmethoxypyridine into diphenylmethyl ethers is described. Several catalytic Lewis acids were screened to obtain better optimal conditions for the formation of diphenylmethyl ether, and the treatment of a variety of alcohol with 2-diphenylmethoxypyridine in the present of small amount of iron could produce the desired diphenylmethyl ethers with high yield. This result will give a potential approach for the practical synthesis of various diphenylmethyl ethers from alcohols.

Poster Presentation : **ORGN.P-194**

Organic Chemistry

Exhibition Hall 2, 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-195**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and Characterization of Novel Histone Deacetylase (HDAC) Inhibitors Containing Biaryl Benzamide Units

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Histone deacetylases (HDACs) are enzymes that play a crucial role in gene expression regulation and cell state. It was known that inhibition of histone deacetylases (HDACs) is associated with cell differentiation, growth arrest, or apoptosis of tumor cell lines as well as the regulation of metabolism. Thus the study of HDACs is important approach to find potential novel anticancer agents. So far several types of HDAC inhibitors such as hydroxamic acid-type HDAC inhibitors and benzamide-type HDAC inhibitors have been developed for the treatment of cancers. Herein, modification of chemical structures at zinc binding domain group and the cap group of benzamide structure was performed to yield potential HDAC inhibitors, and mono-fluoro group was inserted into biaryl benzamide derivatives. And then the characterizations of newly prepared HDAC inhibitors were investigated to see the possibility of application into animal study.

Poster Presentation : **ORGN.P-196**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Properties of polymers based on thiazolo[5,4-b]pyridine as electron-withdrawing unit applied to the flexible polymer solar cell

Juwon Kim, Hongsuk Suh^{1,*}

Chemistry, Pusan National University, Korea

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

Environment problems like fossil fuel exhaustion have been recognized as one of the most serious problems. Polymer solar cell (PSC) using solar energy generation is green and renewable energy because of their advantages. It doesn't have a smoke and also has low cost, light-weight, easy to flexibility and transparency. We synthesized π -conjugated polymers based on pyridine to use for PSC including electron-withdrawing groups (EWG), 2-{3-[4,6-bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-b]pyridine (mTP), and confirm the properties of position of functional group. π -Conjugated polymers, mPTPBDT-EH, mPTPBDTT-EH and mPTPPTI, were based on 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 rich units and mTP as EWG. The device including mPTPPTI showed a VOC of 0.72 V, a JSC of 4.95 mA/cm², and a FF of 0.32, giving a PCE of 1.15%.

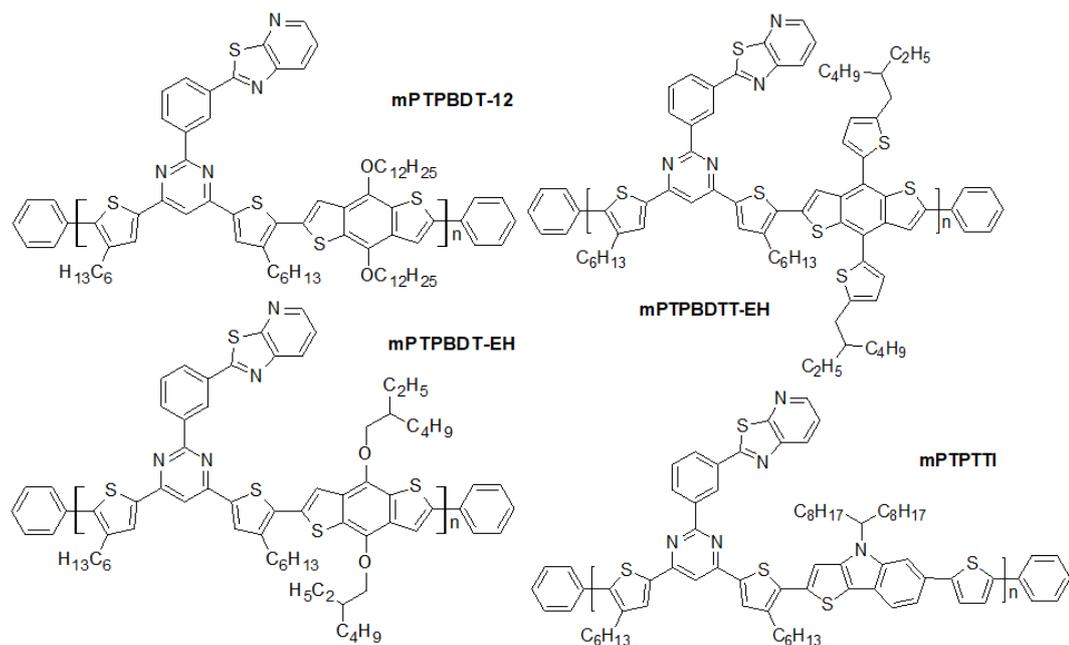


Figure 1. The design of the monomers



Poster Presentation : **ORGN.P-197**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

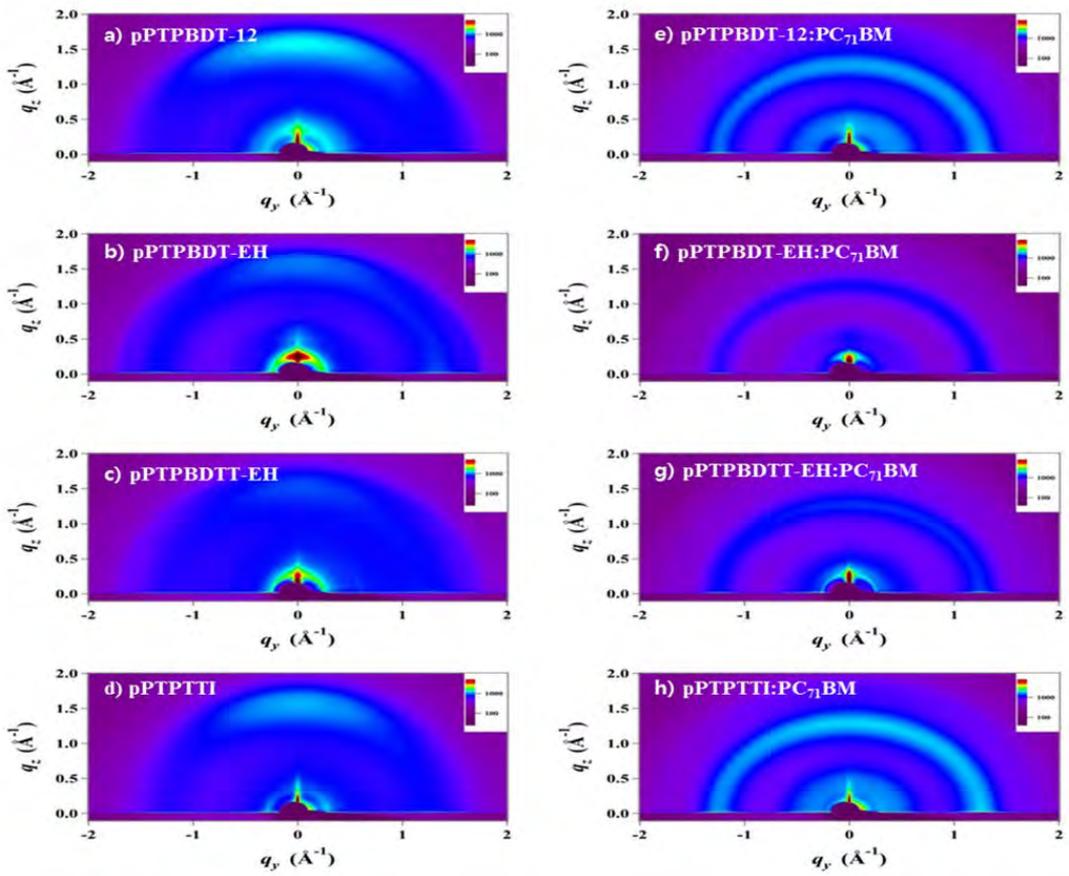
Property of thiazolo[5,4-b]pyridine as electron-withdrawing groups in the polymer solar cells

Juwon Kim, Hongsuk Suh^{1,*}

Chemistry, Pusan National University, Korea

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

Polymer solar cells (PSCs) are attracting attention as a solution to the coming energy crisis in terms of converting solar energy into electrical energy. Compared to many other types of solar cells, PSCs has economic and practical potential due to their flexibility and various synthesis strategies. Polymers, pPTPBDTT-EH, pPTPTTI, pPTPBDT-EH were comprised of 4,8-bis(5-thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene (BDTT), or 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI), or benzo[1,2-b:3,4-b']dithiophene (BDT), as electron-donating groups and 2-{4-[4,6-bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-b]pyridine (pPTP) as electron-accepting groups was made. Herein, pPTP is a newly designed material for the purpose of a novel electron-deficient units in the polymer solar cells and located at the para site of the pyrimidine backbone. Among the designed polymers, pPTPTTI showed the highest efficiency. The device was comprised of pPTPTTI and PC71BM (1:1) with 3% CN additive indicated a fill factor (FF) of 0.31, a JSC of 4.41 mA/cm², a VOC of 0.83 V, showing a power conversion efficiency of 1.13%.



Poster Presentation : **ORGN.P-198**

Organic Chemistry

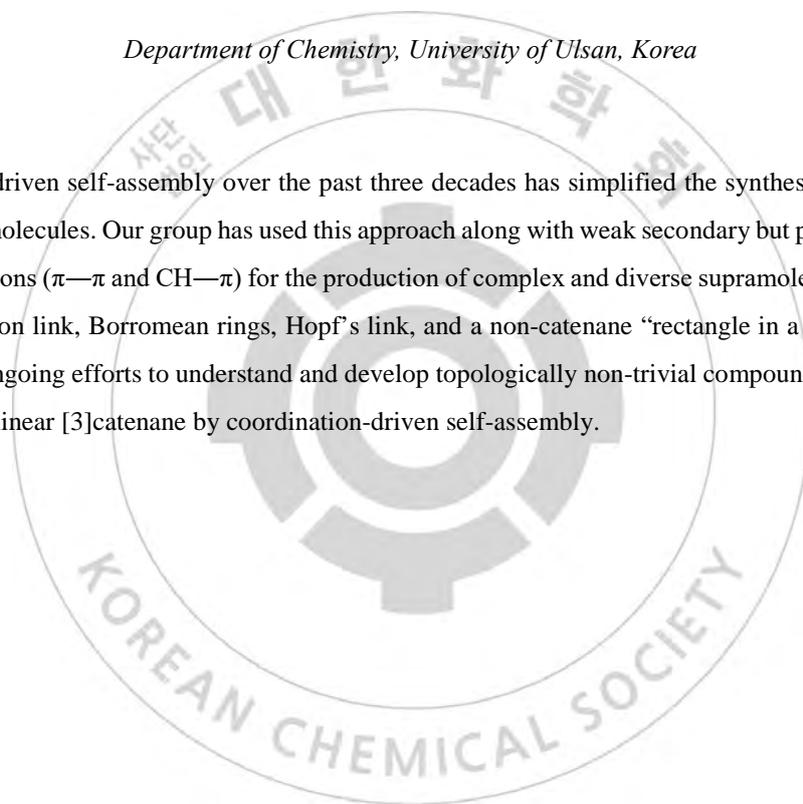
Exhibition Hall 2, THU 11:00~12:30

Coordination-driven self-assembly of a linear [3]catenane

Jatinder Singh, Dong Hwan Kim, Ki-Whan Chi*

Department of Chemistry, University of Ulsan, Korea

Coordination-driven self-assembly over the past three decades has simplified the synthesis of various 2D and 3D supramolecules. Our group has used this approach along with weak secondary but pivotal inter/intra cyclor interactions ($\pi-\pi$ and $\text{CH}-\pi$) for the production of complex and diverse supramolecular topologies such as Solomon link, Borromean rings, Hopf's link, and a non-catenane "rectangle in a rectangle". As a result of our ongoing efforts to understand and develop topologically non-trivial compounds, we report the synthesis of a linear [3]catenane by coordination-driven self-assembly.



Poster Presentation : **ORGN.P-199**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Single Crystal X-ray Structures of Coordination-driven Self-Assemblies

Dong Hwan Kim, Ki-Whan Chi*

Department of Chemistry, University of Ulsan, Korea

In recent years, coordination-driven self-assembly has become a dominant method for constructing 2D and 3D supramolecular architectures. These supramolecular architectures are fascinating not only because of their structural beauty and topological importance but also because of their application in catalysis, host-guest chemistry, molecule recognition, and drug-delivery. Our group has reported a number of complex supramolecular topologies such as [2]catenane or Hopf link, Solomon links, Borromean rings, ring-in-ring and very recently a molecular knot 8_{18} using this method. Due to the structural complexity, determination of structure by conventional spectroscopic techniques is not possible, therefore, single-crystal X-ray analysis remains the only technique to establish the structure. Suitable single crystals for X-ray diffraction analysis were obtained by the vapor-diffusion method. Coordination-driven self-assembly of tetracene-based Ru(II)-acceptor and 1,4-bis(4-pyridylethynyl)tetrafluorobenzene donor along with the non-covalent interactions ($\text{CH}\cdots\pi$ and $\pi-\pi$) results in the formation of a molecular Borromean ring, as revealed by synchrotron X-ray diffraction analysis (Fig 1). After establishing the solid-state structure, other complementary spectroscopic techniques such as ^1H NMR, ^{13}C NMR, and DOSY, along with ESI-MS and elemental analysis were used to fully establish the structure in solid as well in solution state.

Poster Presentation : **ORGN.P-200**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Phosphorus (V) oxychloride-Mediated Synthesis of *N*-Aryl-Substituted Azacycles from Cyclic Ethers

Minh Thanh La, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

N-Substituted azacycles is currently an important structure in organic chemistry and medicinal chemistry area. Many natural products including vitamins, alkaloids, and hormones, and drugs such as Pibrentasvir, Brigatinib, and Gilteritinib contain *N*-substituted azacycle moiety in their structure. Thus, several synthetic methods have been developed to prepare *N*-substituted azacycle compounds. In additions, recently several metal-based synthetic methods were reported. Herein, a practical protocol for the preparation of *N*-aryl substituted azacycles has been described. In this method, five- and six-membered azacycles are synthesized by the reaction of arylamines and cyclic ethers in the presence of phosphorus (V) oxychloride. Utilizing this procedure, a series of *N*-aryl substituted pyrrolidines, 2-methylpyrrolidines, piperidine, isoindolines, and tetrahydroisoquinolines are readily obtained in high yields. This efficient protocol provides a metal-free synthetic approach for the synthesis of *N*-aryl substituted azacycles from cyclic ethers.

Poster Presentation : **ORGN.P-201**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Nickel-catalyzed decarboxylative coupling reactions for the synthesis of 1,3-enynes

SeHyeon Han, Beomseok Ryu, Sunwoo Lee^{1,*}

Chonnam National University, Korea

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

1,3-Enyne is important moiety in pharmaceutical and material chemistry. A number of synthetic methods for 1,3-enyne has been developed including hetero cross dimerization of alkynes. However, gem-selective cross dimerization of alkynes which is formed through head-to-tail cross coupling has been limited to precious metal catalysts and terminal alkynes.¹ We developed that the reaction of alkynoic acid and terminal alkyne with 20 mol% NiCl₂·6H₂O/CuI in TMEDA provided the decarboxylative dimerized product 1,3-enyne instead of 1,3-diyne. This reaction system is mild and showed good in regioselectivity and functional group tolerance.

Poster Presentation : **ORGN.P-202**

Organic Chemistry

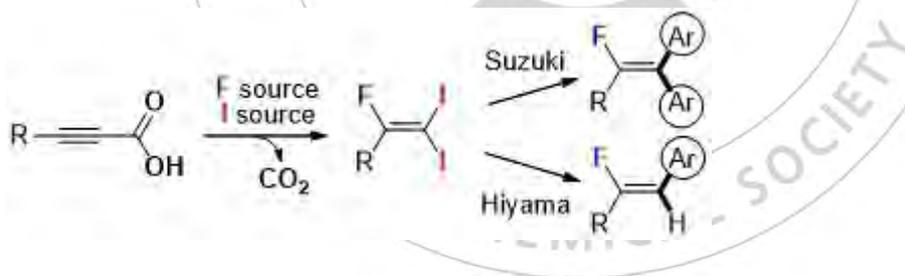
Exhibition Hall 2, THU 11:00~12:30

Synthesis of 1-Fluoro-2,2-diiodovinylarenes via Decarboxylation of Alkynoic Acids and Their Coupling Reactions

Aravindan Jayaraman, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

We developed a method for the synthesis of 1-fluoro-2,2-diiodovinylarene derivatives from alkynoic acids. A variety of aryl alkynoic acids reacted with 1,3-diiodo-5,5-dimethylhydantoin (DIH) in the presence of HF·pyridine to provide the corresponding 1-fluoro-2,2-diiodovinylarenes in good yields. This reaction has a high degree of functional group tolerance and is carried out under mild conditions. In addition, Pd-catalyzed cross-coupling reaction of the synthesized 1-fluoro-2,2-diiodovinylarenes afforded diaryl coupling products in the Suzuki reaction and mono-aryl coupling products in the Hiyama reaction.



Poster Presentation : **ORGN.P-203**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

ElectroChemical Synthesis of β -Amidovinyl Sulfone from Aryl Sulfonylhydrazide and Tertiary Amine

Han-Sung Kim, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

The synthesis of vinyl sulfones has aroused great interest because of their biological activities such as inhibitors of enzymes and important intermediates for the synthesis of organic compounds. Taking into account the importance of vinyl sulfones, we need to develop more synthetic methods to satisfy the need for such compounds. Herein, we introduce the aerobic oxidative reaction of aryl sulfonylhydrazides with tertiary aliphatic amines to form the corresponding vinyl sulfones in the presence of electrochemical conditions. This method provides a mild, practical, and environmentally friendly procedure to synthesize vinyl sulfones in good to moderate yields.



Poster Presentation : **ORGN.P-204**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Systematic Comparison Study on Emission Behaviour of Old and New Fluorophores: The Cellular Environment, the Third Space for Fluorophores

Ye Jin Reo, Kyo Han Ahn*

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

Microscopic imaging aided with fluorescent probes is essential in studying biological systems. Through ratiometric imaging, it is even able to extract quantitative information on a target analyte in cell and tissue. However, in the data extraction process, usually researchers resort to the fluorescent properties of probe and probe-analyte complex obtained in solutions, not in actual microenvironment. As fluorescence signals are environment-sensitive, a possible gap between the “in solution” and “in cellulo” fluorescence characterization data would undermine the reliability of the information extracted. Herein, we disclose a systematic comparison study on the fluorescent properties of commonly-used and new fluorophores in solutions and in cells. The fluorophores showed distinct emission intensity patterns in all of the three media, which underlines that neither the organic or aqueous buffer can mimic the cellular environment. With the course of systematic study on the fluorescence characteristics in the cellular environment, we also report a fluorophore, a benzo[g]coumarin derivative, which is exceptionally bright inside cells and also its emission wavelength is relatively environment-insensitive. To demonstrate the advantage of the environment-insensitive fluorophores for obtaining reliable quantification data, the intracellular hydrogen peroxide level was investigated using the ratiometric probe developed based on the benzo[g]coumarin derivative in four different cell lines. The results documents a robust ratiometric imaging technique aided with environment-insensitive fluorescent probes for in cellulo quantification of biological molecules.

Poster Presentation : **ORGN.P-205**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthetic studies toward frutescone O and Menaquinol-7

Seewon Joung

Department of Chemistry, Mokpo National University, Korea

Frutescone natural products has been isolated from eastern Asian herb *Baeckea frutescens*. Recently, frutescone H-R was isolated along with the potent anti-inflammatory activity. Frutescone O possess most promising activity but it has never been synthesized yet. Synthetic study for this natural product will lead us to a new class of anti-inflammatory drug candidates. Frutescone O has tetracyclic structure including a spirocarbon and a cyclopropane. Proposed biosynthetic pathway suggest that the tasmanone derivative and the sabina ketone derivative would be a good candidates of the key fragments for the total synthesis. To achieve the fragment syntheses, we will develop practical synthesis of (-)-sabina ketone and enantioselective alkylation of conjugated sulfone.

Menaquinol-7(MK-7) is a derivative of Vitamin K. MK-7 has been used as a food additives that is known to be good for osteoporosis and cardiovascular disease. There is no effective chemical synthesis yet. Scalable synthesis of MK-7 would provide efficient production of the valuable food additive as well as interesting synthetic pathway for polyprenyl alcohol.

Poster Presentation : **ORGN.P-206**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

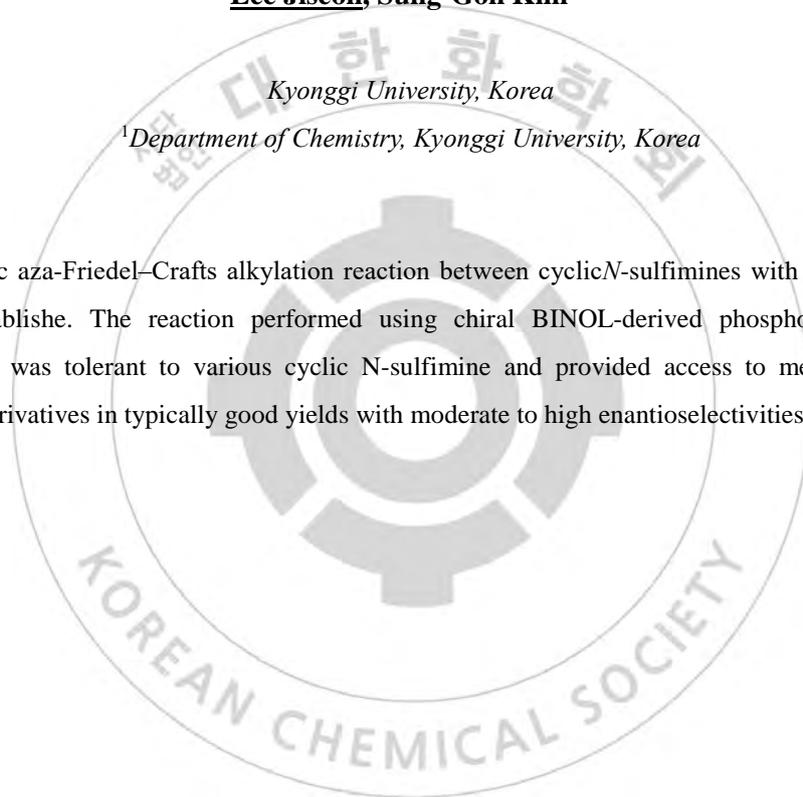
Asymmetric Phosphoric Acid-Catalyzed Aza-Friedel–Crafts Reaction of Furan with Cyclic *N*-Sulfines

Lee Jiseon, Sung-Gon Kim^{1,*}

Kyonggi University, Korea

¹*Department of Chemistry, Kyonggi University, Korea*

An asymmetric aza-Friedel–Crafts alkylation reaction between cyclic *N*-sulfines with 2-methoxyfuran has been established. The reaction performed using chiral BINOL-derived phosphoric acid as an organocatalyst was tolerant to various cyclic *N*-sulfines and provided access to methoxyfuran-2-yl sulfamidate derivatives in typically good yields with moderate to high enantioselectivities (up to 94:6 er).



Poster Presentation : **ORGN.P-207**

Organic Chemistry

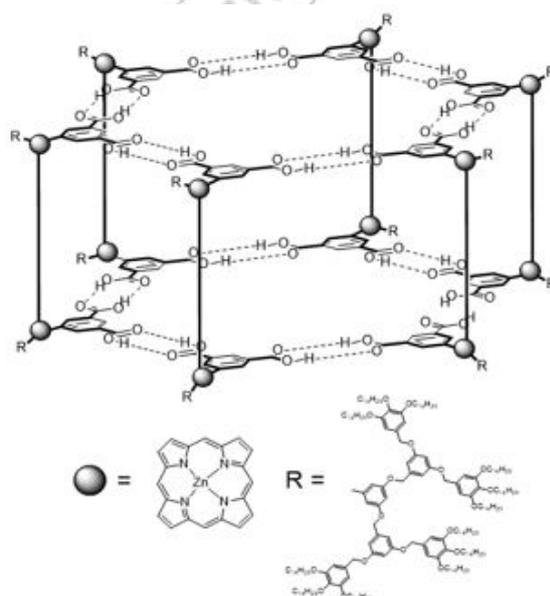
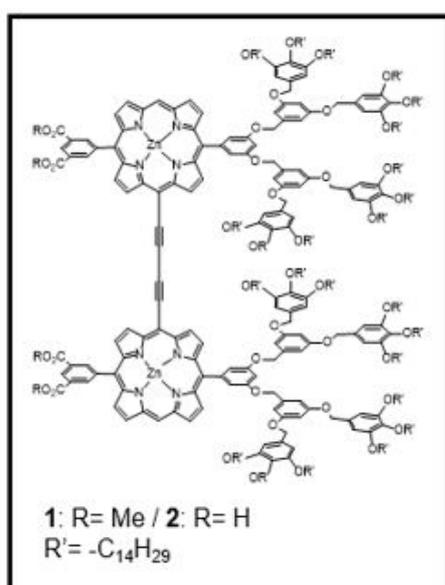
Exhibition Hall 2, THU 11:00~12:30

Hydrogen bonding mediated Hexameric self-assembly of porphyrin dimer

Hyun Jun Park, Hosoo Lee, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

We design hydrogen bonding mediated hexameric self-assembly with butadiyne linked Zinc porphyrin dimer as a building block. We introduced four carboxylic acid groups and dendritic units to Zinc porphyrin dimer for constructing self-assembly and enhanced solubility, respectively. We confirmed assembling phenomenon with UV-Vis absorption spectrum. $P_{Zn}-CO_2Me$ (**1**) and $P_{Zn}-COOH$ (**2**) show different UV-Vis absorption in various solvents. **1** shows comparative similar absorption in various solvents but **2** doesn't. Furthermore, **2** UV absorption significantly change in chloroform after 7 days. But in 1,4-Dioxane that can compete with **2** in hydrogen bonding, there is no prominent change. For more intuitive and quantitative measurement, we collect other data. Detailed aspect of this system will be reported in the symposium.



Poster Presentation : **ORGN.P-208**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Asymmetric Friedel–Crafts Reaction of 3-Indolylsulfamidates with Indoles for the construction of enantioenriched bisindolylmethane sulfamates

Yerin Kim, Sung-Gon Kim^{1,*}

Kyonggi University, Korea

¹*Department of Chemistry, Kyonggi University, Korea*

A Brønsted acid-catalyzed asymmetric Friedel–Crafts alkylation of 3-indolylsulfamidates with indoles has been established toward the efficient synthesis of biologically important bisindolylarylmethane derivatives containing the phenylsulfamate group. The reaction using chiral BINOL-derived phosphoric acid as the catalyst was tolerant to a diverse range of 3-indolylsulfamates and indoles, and provided for the first time bisindolylarylmethane sulfamate derivatives in good yields and with moderate to high enantioselectivities (up to 89% yield, 94:6 er).

Poster Presentation : **ORGN.P-209**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Asymmetric [3+3] cycloaddition of donor–acceptor aziridines with *N,N*-dialkyl-3-vinylanilines for the stereoselective synthesis of highly functionalized enantioenriched tetrahydroisoquinolines

Kim Seungyeon, Yong Il Kwon¹, Sung-Gon Kim*

Department of Chemistry, Kyonggi University, Korea

¹*Kyonggi University, Korea*

A diastereo- and enantioselective [3+3] cycloaddition of donor–acceptor aziridines with *N,N*-dialkyl-3-vinylanilines has been established using a Mg(OTf)₂/bisoxazoline catalyst, providing highly functionalized tetrahydroisoquinolines in good yields and with high levels of stereocontrol. A wide variety of *N,N*-dialkyl-3-vinylanilines, such as *m-N,N*-dimethylaminophenyl α,β -unsaturated phenyl ketones and 3-(*m-N,N*-dimethylaminophenyl)acrylates, as well as donor–acceptor *N*-tosylaziridines, have been applied in this asymmetric catalytic protocol.

Poster Presentation : **ORGN.P-210**

Organic Chemistry

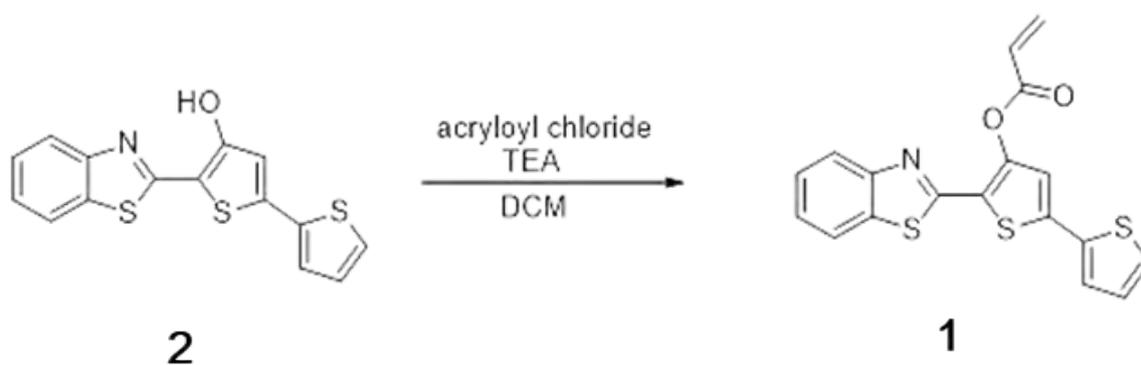
Exhibition Hall 2, THU 11:00~12:30

Fluorescence Probe based on ESIPT: Selective Detection of Cysteine existed in Mitochondria

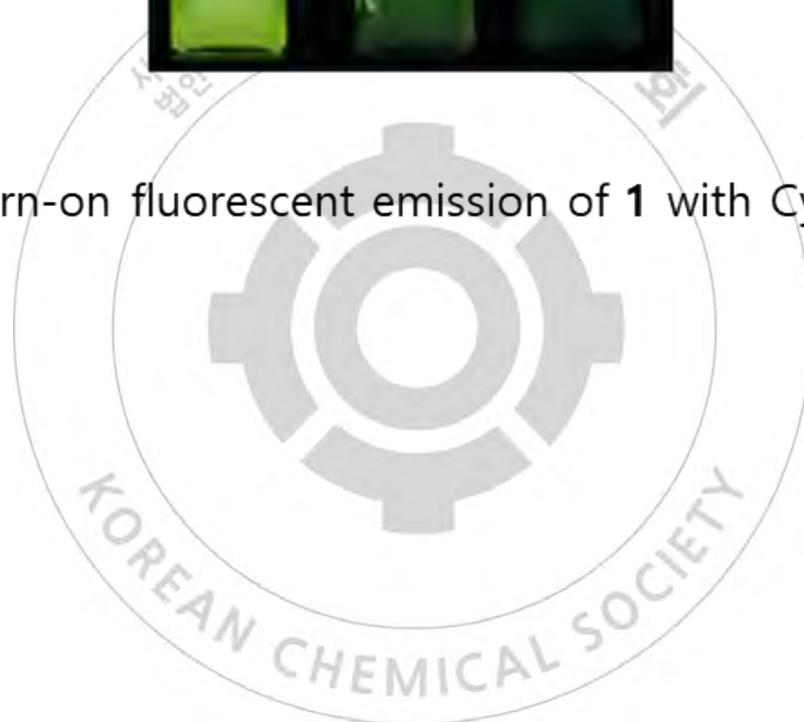
Kyeong-Im Hong, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Intracellular thiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) play important roles in biological system. For example, Cysteine in mitochondria is associated with the process of mitochondrial protein turnover and maintaining ROS levels. However, cysteine is associated with many diseases such as liver damage, cancer, and Alzheimer's disease. Therefore, the development of fluorescent probe for cysteine is necessary due to their high sensitivity and selectivity. We have designed fluorescence probe (**1**) for selective detection of cysteine. We have reported ESIPT based fluorescent probe (**2**) for mitochondria visualization. **2** was reacted with acryloyl chloride to obtain **1**. The fluorescent emission of **1** was increased by cysteine over GSH and Hcy. The probe, **1**, could efficiently recognize cysteine in mitochondria of living cell. Detailed aspect of this system will be discussed in this symposium.



Turn-on fluorescent emission of 1 with Cys



Poster Presentation : **ORGN.P-211**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

[Withdrawal] Interfacial Photopolymerization by Xanthene Dyes towards Colorimetric Detection

Young Jae Jung, JungKyu Lee*

Department of Chemistry, Kyungpook National University, Korea



Poster Presentation : **ORGN.P-212**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

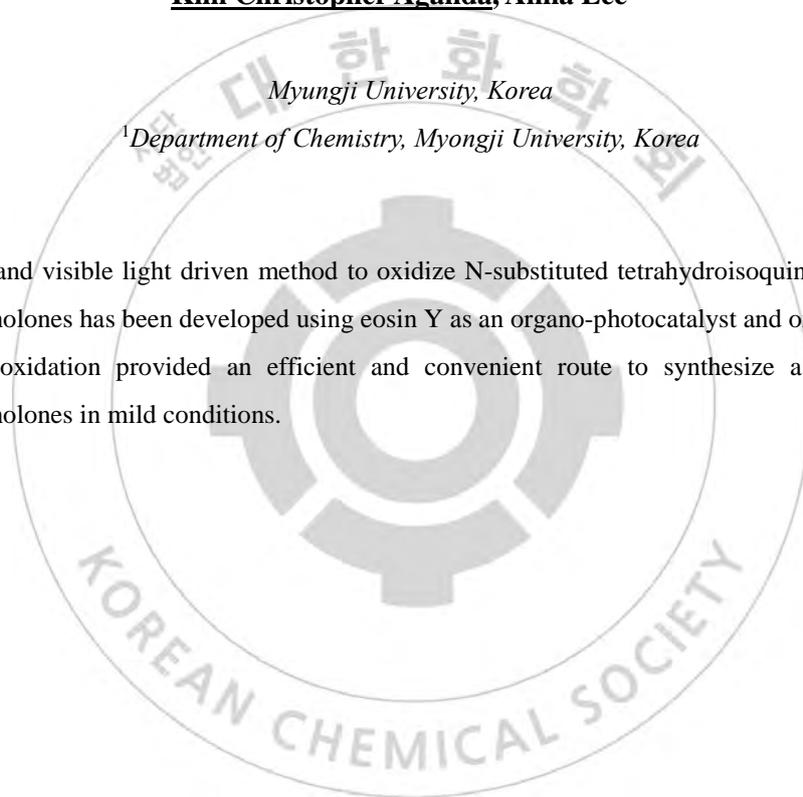
Aerobic α -Oxidation of N-Substituted Tetrahydroisoquinolines to Dihydroisoquinolones

Kim Christopher Aganda, Anna Lee^{1,*}

Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

A metal free, and visible light driven method to oxidize N-substituted tetrahydroisoquinoline (THIQ) to dihydroisoquinolones has been developed using eosin Y as an organo-photocatalyst and oxygen as a green oxidant. The oxidation provided an efficient and convenient route to synthesize a wide range of dihydroisoquinolones in mild conditions.



Poster Presentation : **ORGN.P-213**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Efficient preparation method of 4-hydroxybenzoic esters – Oxidation of substituted Hagemann's ester

Aleksei Golikov, Dahye Kim¹, Sangho Koo^{2,*}

Department of Chemistry, Myungji University, Korea

¹*Department of Energy Science and Technology, Myungji University, Korea*

²*Department of Chemistry, Myungji University, Korea*

Herein, we obtained R-substituted 4-hydroxybenzoic esters by applicable method. Initially, two equivalents of ethyl acetoacetate were coupled with various aliphatic aldehydes in t-BuOK/t-BuOH to receive appropriate Hagemann's esters in high yields. Further reaction utilizing stoichiometric NBS as an oxidizing reagent and catalytic TMS-OTf permits the preparation of medicinally and industrially useful 4-hydroxybenzoic esters.



Poster Presentation : **ORGN.P-214**

Organic Chemistry

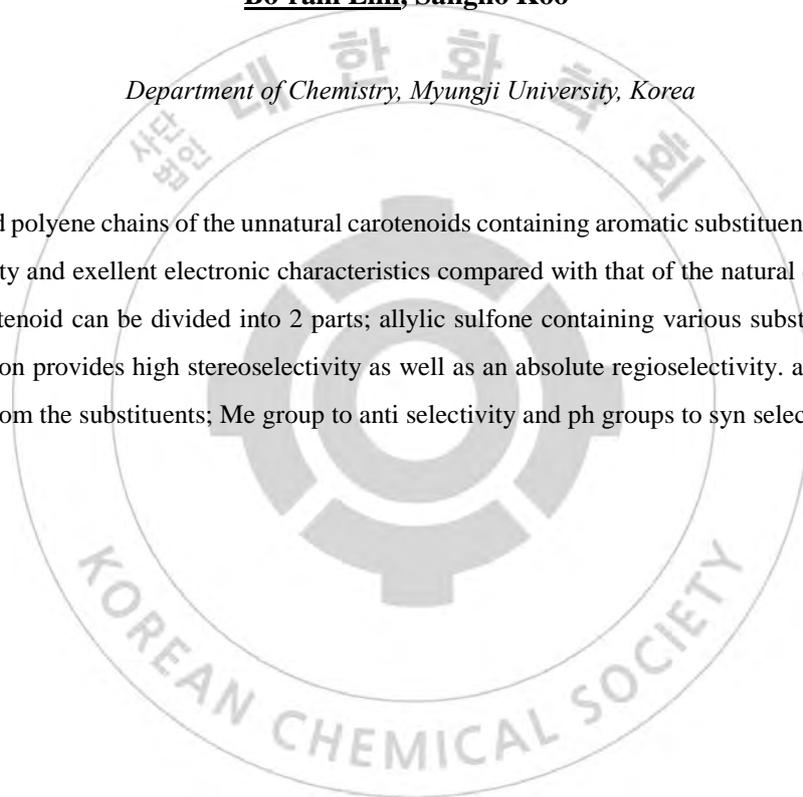
Exhibition Hall 2, THU 11:00~12:30

Synthesis of efficient units for the carotene wire containing phenyl substituents.

Bo-ram Lim, Sangho Koo*

Department of Chemistry, Myungji University, Korea

The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would provide an extra stability and excellent electronic characteristics compared with that of the natural carotenoids. The unnatural carotenoid can be divided into 2 parts; allylic sulfone containing various substituents and dial unit. The reaction provides high stereoselectivity as well as an absolute regioselectivity, and the selectivity is originated from the substituents; Me group to anti selectivity and ph groups to syn selectivity.



Poster Presentation : **ORGN.P-215**
Organic Chemistry
Exhibition Hall 2, THU 11:00~12:30

Heterocyclic Compounds Generation by using Mn(III)/Co(II) Catalyzed Oxidative Deacetylation

Tingshu Wang, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

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. We found a new type of hetero-cyclization directed by a 1,4-dicarbonyl compound. Based on the above oxidation, a high yield of oxidative deacetylation was gained under the combined catalyze of Mn(AcO)₃ and CoCl₂. Using this method, the starting material for one pot syntheses of multi-substituted furan, thiophene, and pyrrole were easily gained. Further work on extending this catalytic oxidative reaction to the synthesis of some natural products is ongoing.

Poster Presentation : **ORGN.P-216**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Fast Assembly and High-Throughput Screening of Structure and Antioxidant Relationship of Carotenoids

Dahye Kim, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Carotenoids generally contain conjugated carbon-carbon double bonds which endow the red pigments with light harvesting and energy transferring abilities as well as antioxidant activity by scavenging reactive oxygen species (ROS). It was envisioned that the structural modification of the terminal rings would significantly alter the effective conjugation and, thus, the reactivity of the conjugated polyene chain toward ROS. Novel C₂₀ heptaenyl diphosphonate was devised to facilitate one-pot synthesis of various carotenoids. Olefination with diversely substituted aromatic aldehydes allowed fast assembly of the corresponding carotenoids. The structure and activity relationship (SAR) of carotenoids was investigated by high-throughput screening (HTS) of ABTS and DPPH assays and their hierarchical clustering analysis. Antioxidant activity of carotenoids increased with the number of electron-donating substituents. Carotenoid with multiple electron-donating substituents was most proficient, which showed better radical scavenging activities than β -carotene and lycopene.

Poster Presentation : **ORGN.P-217**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

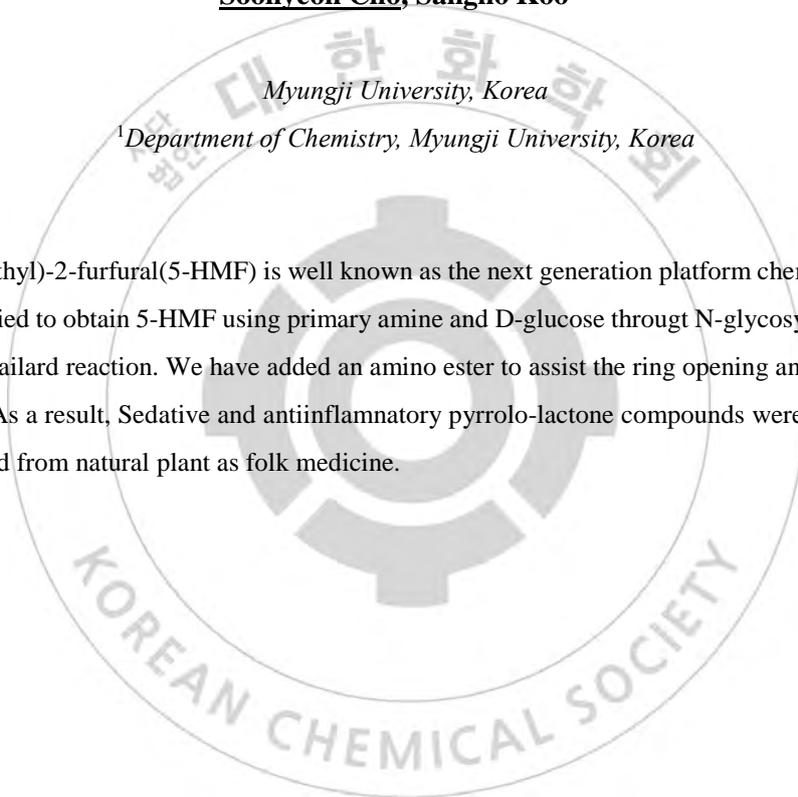
One-pot Synthetic methods from Reducing Sugar to Pyrrolo-lactone compound.

Sooheon Cho, Sangho Koo^{1,*}

Myungji University, Korea

¹*Department 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-218**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

High Throughput Screening of Structure and Antioxidant Relationship of Carotenoids.

Gaosheng Shi, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

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-219**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of unnatural carotenoids with good electrical properties

Huijung Yang, Sangho Koo^{1,*}

Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Carotenoids have a variety of beneficial effects and are particularly good at antioxidant activity. unnatural carotenoids substituted with phenyl groups have good electrical properties in addition to their advantages. Using these advantages, the electrical conductivity can be measured by replacing the terminal group with a methylthio group and attaching to the gold plat. This unnatural carotenoids can be efficiently synthesized by the julia-kocienski olefination of triene dialdehyde with BT(benzothiazole)-Sulfone. It can assemble the methylthio group through a wittig reaction with 4-thiomethylbenzyl phosphonium bromide.

KOREAN CHEMICAL SOCIETY

Poster Presentation : **ORGN.P-220**

Organic Chemistry

Exhibition Hall 2, 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, Korea

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-221**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Investigation of Hypervalent λ^3 - and λ^5 -Aryliodines as ^{18}F -Labeling Precursors to Produce $[^{18}\text{F}]$ Aryl Fluorides

Young-Do Kwon, Jeongmin Son¹, Young hoon Ryu, Joong-Hyun Chun*

Department of Nuclear Medicine, Yonsei University College of Medicine, Korea

¹Department of Nuclear Medicine, Yonsei University Health System, Korea

Positron emission tomography (PET) provides useful biological information in a non-invasive manner. To take advantage of this benefit in a clinical application, new radiochemical methodology needs to be avidly developed, particularly to incorporate fluorine-18 onto aromatic chemical entity. Among the newly developed methods, the use of hypervalent aryliodines, such as diaryliodonium salts and iodonium ylides, as labeling precursors has drawn significant attention in ^{18}F -PET radiochemistry. Recent report on oxidized iodoarenes (OIAs) as an expedient ^{18}F -labeling precursor opens up the practical and convenient route to produce $[^{18}\text{F}]$ fluoroarenes in clinical setting. However, it is still obscure that which hypervalent species is the major component functioning as an active precursory role during radiofluorination. Herein, we investigated the labeling efficacy of different λ^3 - and λ^5 -oxidized hypervalent aryliodines as precursors to produce no-carrier-added $[^{18}\text{F}]$ aryl fluorides. Interestingly, λ^3 -hypervalent iodosyl and benziodoxole derivatives provided $[^{18}\text{F}]$ fluorobenzene in 32 and 13% RCYs, which are new entries as labeling precursors for the reaction with cyclotron-produced $[^{18}\text{F}]$ fluoride ion. These higher-valent iodoarenes may provide an efficient route to the production of aromatic PET radiotracers for application in molecular imaging. This work was supported by the National Research Foundation (NRF) of Korea, funded by the Ministry of Science (NRF-2015R1D1A1A02061420).

Poster Presentation : **ORGN.P-222**

Organic Chemistry

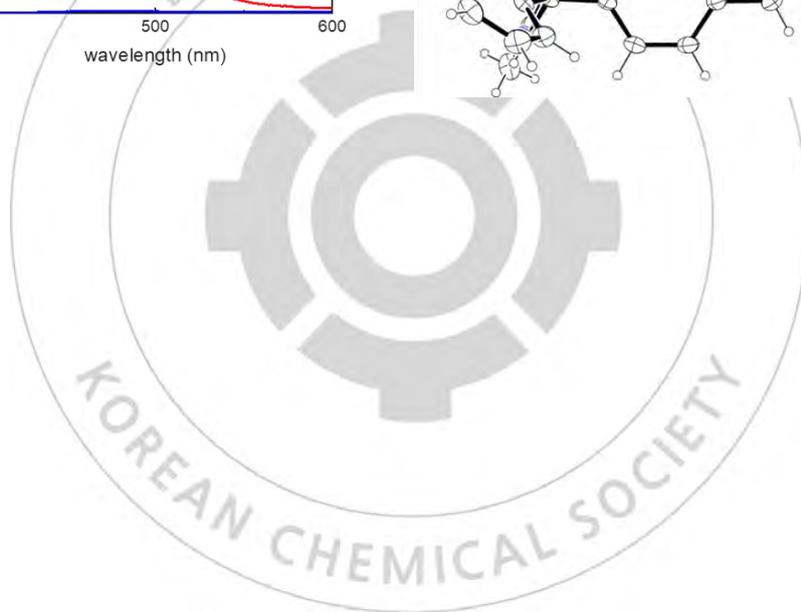
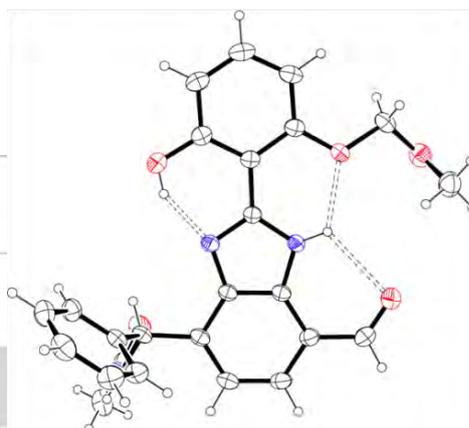
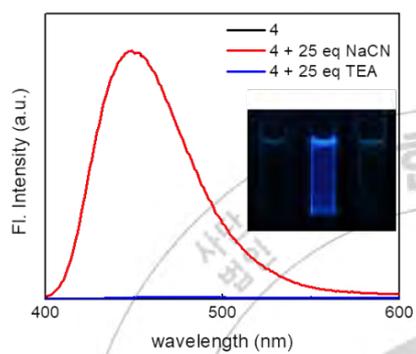
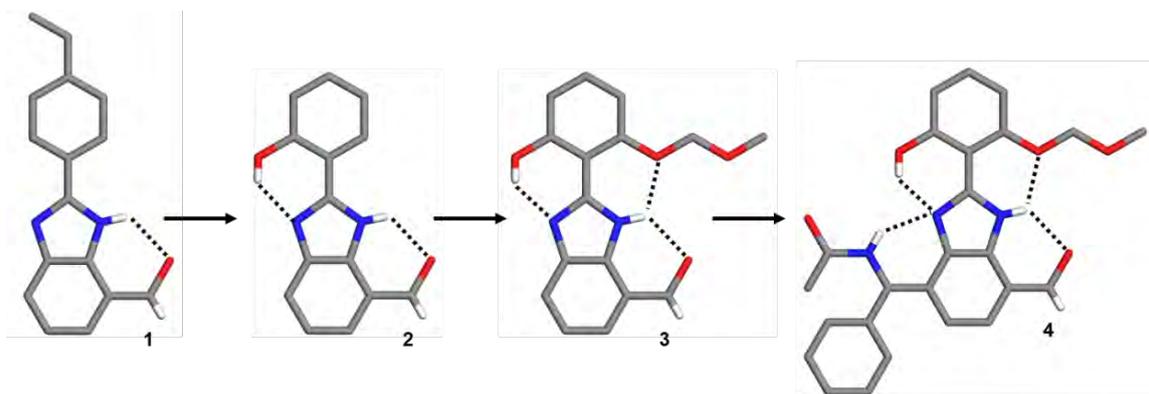
Exhibition Hall 2, THU 11:00~12:30

Structural Tuning of Biomimetic Hydrogen Bonding and Tautomer Equilibrium for Reaction-Based Fluorescence Turn-On Detection of Cyanide Ion

Hyunchang Park, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Hydrogen bonding, a prominent class of supramolecular interactions, has been used extensively as key functional components for molecular assembly, activation, and signaling. Among a wide range of donor–acceptor structural motifs used for hydrogen bonding, imidazole possesses unique features: 1) capability to function as both hydrogen bonding donor and acceptor, 2) interconversion between donor and acceptor through tautomerization. Utilizing the distinctive functionality of imidazole, we have designed new molecular probes for covalent capture and fluorescence turn-on detection of toxic cyanide anion. The intramolecular hydrogen bonding mediated by imidazole motif was anticipated to facilitate the bond-forming reaction between nucleophilic cyanide anion and electrophilic aldehyde group that also serves as an internal fluorescence quencher. With insufficient strength of the hydrogen bonding, however, competition with undesired Brønsted acid–base chemistry compromised the overall performance of sensory response. We have thus made systematic variations on the hydrogen bonding donor and acceptor groups around the imidazole core to control the strength of the hydrogen bonding and to regulate the tautomer equilibrium. The most advanced system **4**, optimized through the iterative design process, displayed highly sensitive, selective, and rapid fluorescence turn-on response to cyanide ion. A combination of spectroscopic, X-ray crystallographic, and kinetic studies point toward a coherent mechanistic model, which will be discussed in detailed in this presentation.



Poster Presentation : **ORGN.P-223**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis, Crystal Structure and Hirshfeld Surface Analysis of 1,2-bis(2',6'-diisopropoxy-[2,3'-bipyridin]-6-yl)benzene

Suk-Hee Moon, Youngjin Kang^{1,*}, Ki-Min Park^{2,*}

Department of Food & Nutrition, Kyungnam College of Information & Technology, Korea

¹*Division of Science Education, Kangwon National University, Korea*

²*Research Institute of Natural Science, Gyeongsang National University, Korea*

In order to achieve blue phosphorescent materials, the design of ligands with a large triplet energy needs to be taken into account as the first step. Our interest in the preparation of phosphorescent metal complexes has been focused on the development of a suitable tetradentate ligand based on 2,3'-bipyridine with a large triplet energy. Moreover, the crystal structures of 2,3'-bipyridine-based tetradentate molecules have aroused our curiosity, because the knowledge of the coordination modes to a metal ion are of paramount importance in understanding its chemical and physical properties. 1,2-bis(2',6'-diisopropoxy-[2,3'-bipyridin]-6-yl)benzene (**L**), as a tetradentate molecule with a large triplet energy displays a helical structure induced by the combination of the C—C—C torsion angle [10.8 (2)°] between two 2,3'-bipyridyl units attached to the 1,2-positions of the central benzene ring and consecutive connections between five aromatic rings through the meta- and ortho-positions. Intramolecular C—H... π interactions between a H atom of a pyridine ring and the centroid of another pyridine ring contributes to the stabilization of the helical structure. In the crystal, weak C—H... π interactions link the **L** molecules into a two-dimensional supramolecular network extending parallel to the ac plane, in which the molecules with right- and lefthanded helical structures are alternately arranged. Hirshfeld surface analysis and two-dimensional fingerprint plots indicate that the molecular packing is dominated by van der Waals interactions between neighbouring H atoms, as well as by C—H... π interactions. Herein, we describe the molecular and crystal structures of the compound **L** that can act as a potential tetradentate ligand to various transition metal ions. In addition, the molecular packing of **L** was examined with the aid of a Hirshfeld surface analysis.

Poster Presentation : **ORGN.P-224**

Organic Chemistry

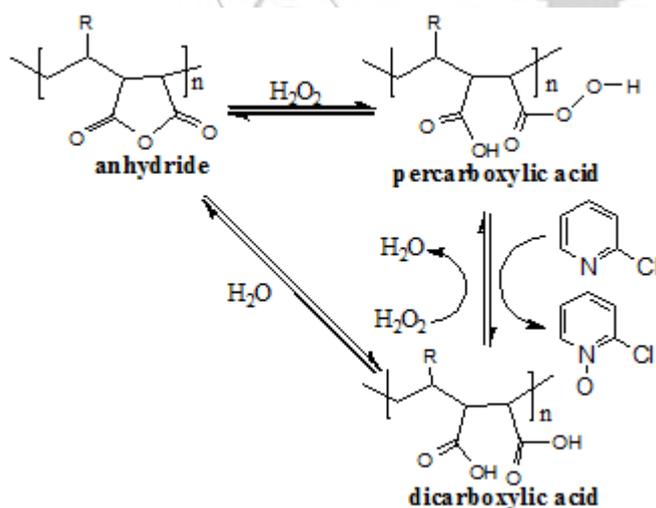
Exhibition Hall 2, THU 11:00~12:30

Green and Recyclable Catalyst for N-oxidation of Pyridine using Hydrogen Peroxide

Sang Hee Lee*, Ghellyn Gajeles, Dong Hee Kim, Se Mi Kim

Department of Chemistry, Kunsan National University, Korea

2-Chloropyridine N-oxide(CPNO), is an important intermediate in the preparation of zinc pyriothione, which is effective as bactericides and fungicides. Because of the electron withdrawing properties of the halogen, 2-chloropyridines can be oxidized with greater difficulty than other pyridine derivatives. The conventional processes for manufacturing CPNO are of multi-steps involving sulfuric acid-catalyzed oxidation of 2-chloropyridine with H₂O₂ as an oxidant, acetic acid, and the separation of CPNO by neutralizing sulfuric acid with sodium hydroxide. In this study, catalytic efficiency and recyclability of poly(α -olefin-co-maleic anhydride) as a reusable organic catalysts will be evaluated in oxidation of 2-chloropyridine to CPNO.



Poster Presentation : **ORGN.P-225**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Synthesis of Degradable Poly (styrene-block-ethylene glycol) with Triarylphosphine by the Staudinger Ligation

Yerin Kim, Myungwoong Kim*, Dong Wook Kim*

Department of Chemistry, Inha University, Korea

Chemoselective ligation has given insight into cellular processes. In order to get selectivity, the two participating functional groups would be abiotic and chemically orthogonal to native cellular components. The Staudinger ligation using azide and triarylphosphine rapidly forms a stable amide bond in the presence of water than unstable aza-ylide hydrolysis product and has high chemoselectivity, mild reaction conditions, non-toxic property as well as nitrogen gas being the only by-product. Through Staudinger ligation, block copolymers having triarylphosphine as a junction point enable to decompose or change one part of block copolymers. Herein we have synthesized degradable block copolymers using polystyrene, methoxy polyethylene glycol(mPEG), and triarylphosphine. The mPEG part in resultant block copolymers was removed by organic azide compounds through Staudinger ligation. The block copolymers were characterized by ¹H NMR and gel permeation chromatography (GPC). The synthesized block copolymers are expected to introduce other functionalized molecules.

Poster Presentation : **ORGN.P-226**

Organic Chemistry

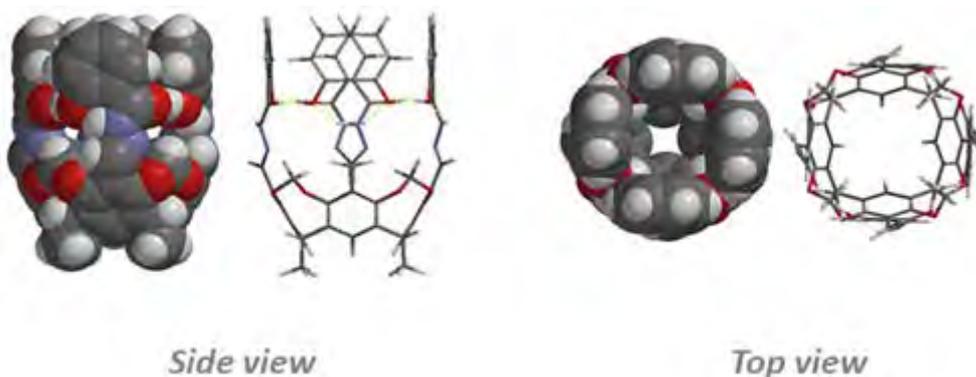
Exhibition Hall 2, THU 11:00~12:30

Complementary binding of self-folding cavitand with 2-hydroxy benzamide moieties

Saegyo Jung, Yeon Sil Park, Kyungsoo Paek*

Department of Chemistry, Soongsil University, Korea

Supramolecules compound with nano-sized inner cavity can be formed when monomer molecules self-assemble. Supramolecules have potentials of utilization on molecular delivery, molecular recognitive system, molecular reaction pot. These functional compound has been interesting issues in supramolecular chemistry. Self-folding cavitands are artificial receptors that are stabilized in their closed, concave conformation by non-covalent interactions. Newly developed self-folding iminocavitand 1 was designed and synthesized by condensation reaction of hydrazide group and well-known resorcin[4]arene cavitand with four formyl groups. The resorcin[4]arene-based cavitand bearing four 2-hydroxy benzamide moieties on the upper rim can enlarged its inner cavity and fold into vase conformer by the four intramolecular C=O...H-O...H-N hydrogen bond sequence in the presence of suitable guests. Self-folding iminocavitand 1 can recognize neutral guest molecules selectively with its inner cavity. Consequently, Supramoleculars with a narrow and deep inner cavity are formed and stabilized, which was confirmed by NMR experiments (1HNMR, 13CNMR, 2D-NOESY NMR) and MALDI-TOF Mass. The synthesis and binding characteristics of this self-folding iminocavitand 1 toward various guests were studied.



Poster Presentation : **ORGN.P-227**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of doubly dendronized polymers with polyglycerol and polylysine dendrons

Gwang Mo Kim, Si Kyung Yang^{1,*}

Chonnam National University, Korea

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

This study describes the design and synthesis of a new class of dendronized polymers. First, high molecular weight polyglycerol dendronized poly(norbornene)s (PGD-PNBs) were synthesized via ring-opening metathesis polymerization of norbornene monomers containing amine functional groups on the side-chains followed by dendron growth from the olefins of PNB backbones using iterative dihydroxylation and allylation. In addition, doubly dendronized polymers that possess two different dendrons, PGDs along the PNB backbone and polylysine dendrons (PLDs) on the side-chains, were designed and synthesized. The surfaces of the PLD and PGD (third-generation for both dendrons) are decorated with 8 amine and 8 hydroxyl groups, respectively. These multiple peripheral groups are useful handles for incorporating additional functionalities such as targeting moieties and fluorophores as well as for making the final structure water-soluble.

Poster Presentation : **ORGN.P-228**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Selective detection of Protein Tyrosine Phosphatase 1B by intrinsic Förster Resonance Energy Transfer (iFRET)

Trishala Durgannavar, Se Jeong Kwon¹, Sang Jeon Chung^{2,*}

Department of Chemistry, Dongguk University, Korea

¹*pharmacy, Sungkyunkwan University, Korea*

²*College of Pharmacy, SungKyunKwan University, Korea*

Protein tyrosine phosphatase 1B (PTP1B) is a validated drug target in several diseases such as type 2 diabetes, obesity, and cancer.¹ Here, a highly selective detection method of native PTP1B is described using a label free Förster resonance energy transfer (FRET) technique. FRET is a distant dependent (10 to 100 Å) photo-physical phenomena where an excited donor fluorophore non-radiatively transfers energy to an acceptor fluorophore. Intrinsic tryptophan residue near the active site of PTP1B serves as the FRET donor and the 1-naphthylamine moiety of the probes act as the FRET acceptor.² Based on a difluoromethylphosphonate phenylalanine tripeptide, a known nanomolar PTP1B inhibitor, and 1-naphthyl-ethylenediamine, several FRET acceptor probes for PTP1B were crafted using solid phase peptide synthesis protocols.³ FRET allowed selective detection of PTP1B was achieved over several other phosphatases, especially the cellular abundant alkaline phosphatases. WPD is a signature motif present in the catalytic site of PTP but absent in alkaline phosphatases which presumably allows selective detection of PTP over alkaline phosphatases. The developed PTP1B probes were found to be competitive inhibitors of purified wild-type PTP1B, our most selective probe was found to have a K_i of about 42 nM ($K_d = 133$ nM). Using our PTP1B probes, an FRET based screening assay of potential PTP1B inhibitors was developed.

Poster Presentation : **ORGN.P-229**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Highly Stereoselective Cyclocarbonylation of Allenyl Glyoxylate: Directed Toward a Synthesis of (+)-Cyclocalopin E

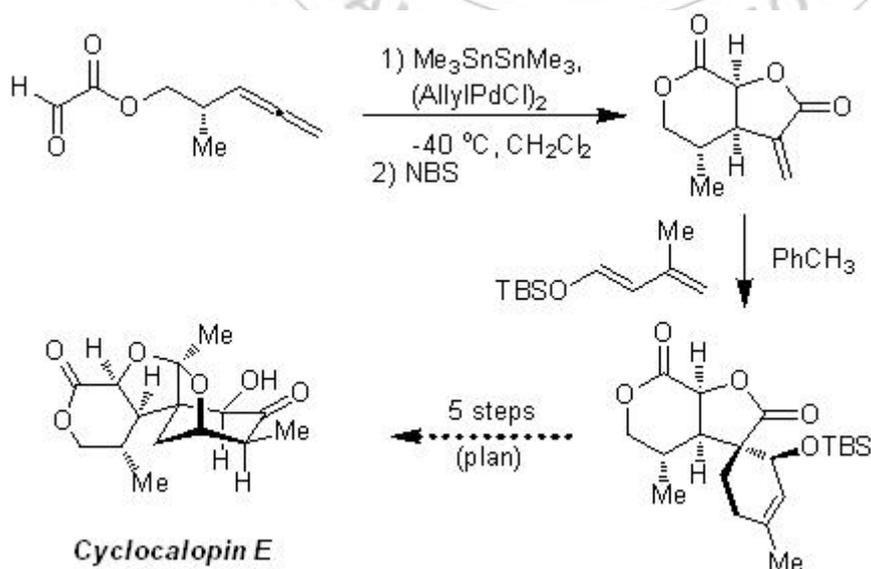
Weonju Yu, Jieun Song¹, Chan-Mo Yu^{2,*}, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

¹*Chemistry Department, Chonnam National University, Korea*

²*Department of Chemistry, Sungkyunkwan University, Korea*

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of transition metals are some of the most attractive methodologies since reactions can directly construct complicate molecules from relatively simple starting materials. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring cyclocalopin series: 1) stereoselective construction of a bis-lactone via direct or stepwise cyclocarbonylation of allenyl glyoxylate ; 2) synthetic studies toward naturally occurring cyclocalopin E.



Poster Presentation : **ORGN.P-230**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Molecular Rotor Probe for Endoplasmic Reticulum Local Viscosity Fluorescence Lifetime Imaging of Reticulophagy

**Jinwoo Shin, Jiseon Kim, Jusung Ahn, Hyeong Seok Kim, Ji Hyeon Kim, Subin Son,
Myung Sun Ji, Wonseok Choi, Jongseung Kim***

Department of Chemistry, Korea University, Korea

Autophagy of the endoplasmic reticulum (ER), termed reticulophagy, is a form of selective autophagy that is linked to the unfolded protein response for maintaining cell homeostasis. Reticulophagy largely contributes to the protein quality control process in the ER; however, the accumulation of unfolded or misfolded proteins in the ER can lead to ER stress, resulting in several pathophysiological processes and severe diseases such as tumorigenesis, neurodegenerative diseases, and diabetes. Therefore, gaining a comprehensive understanding of the reticulophagy process could provide a promising approach for the diagnosis and therapy of these diseases. The current work describes a novel dual-functional fluorescent molecular rotor for imaging ER microviscosity during reticulophagy by a BODIPY-arsenicate fluorophore. The microenvironment-sensitive, dual-functional fluorescent probe 1 was rationally designed to covalently bind to vicinal dithiol-containing proteins (VDPs) in the ER, and thus the selective binding of VDPs in the ER leads to reticulophagy initiation and microviscosity evaluation. Probe 1 was able to induce intracellular reticulophagy while also allowing for quantification of the local viscosity changes of the ER in live cells, thereby providing a quantitative method to monitor the dynamic autophagic processes in the live cells. Due to the molecular rotor (BODIPY) and a phenylarsenicate moiety, we could explore the dynamic changes of the microenvironment in suborganelles during the formation of autolysosome. Furthermore, probe 1 was able to specifically label VDPs in the nascent proteins in the ER, which could result in ER stress because of the accumulation of misfolded or unfolded VDPs. Therefore, probe 1 could be a promising tool for the study of ER autophagy.

Poster Presentation : **ORGN.P-231**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Development of 5-Fluorouracil Derivatives from 5-Fluorouracil

Ha Junghun, Jong Hyun Cho*

Dong-A University, Korea

5-Fluorouracil is an anti-cancer drug currently sold under the name adrucil. It is used as an anti-cancer drug such as breast, stomach, and pancreatic cancer and is used as an intravenous injection method. It is used as an anti-cancer drug, but it has many side effects such as vomiting, diarrhea, headache, hair loss, etc. So we want to develop 5-FU derivative to eliminate side effects and create more stable Substance. The 5-FU works in a variety of ways. However, it serves primarily as an inhibitor for the Thymidylate Synthase (TS). This action blocks the synthesis of pyrimidine and thymidine, also known as nucleoside, making DNA replication impossible. The TS forms the dTMP by methylating the dUMP. However, the 5-FU injection inhibits the dTMP formation and kills the cancer cells. To reduce extreme side effects and to synthesize novel bioactive materials we researched synthesis and development of 5-fluorouracil derivatives from 5-fluorouracil.

Poster Presentation : **ORGN.P-232**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Small molecule-based prodrug for liver cancer therapy

**Myung Sun Ji, Jinwoo Shin, Hyeong Seok Kim, Subin Son, Ji Hyeon Kim, Jusung Ahn,
Jiseon Kim, Jongseung Kim***

Department of Chemistry, Korea University, Korea

In past few years, cancer specific targeted drug formulations have shown some hope of improving the therapeutics with minimized associated side effects of chemotherapy. However, the benefits has proven modest due to lack of systems that can be assessed easily from parent drugs while maintaining the same features of cancer associated prodrug activation. We developed a small molecule-based, carboxylesterase responsive theranostic, EDOX, with tumor-specific enzymatic activation for targeted delivery of the anticancer drug, Doxorubicin (Dox), to hepatocellular carcinoma (HCC) cells. Easy synthetic access, physiological stability, tumor-selective activation, and sustained drug release make EDOX an excellent candidate for use as a next-generation drug delivery system for HCC.

Poster Presentation : **ORGN.P-233**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of 1,3,5-Triazacyclohexanes and Acid-degradable Cationic Polyacrylates as siRNA Delivery Vehicles

Jae Hun Jeong, Soo Kyung Cho^{1,*}

Dong-A University, Korea

¹*Department of Chemistry, Dong-A University, Korea*

There has been a steady study of the drug delivery system within the human body. Among them, efforts to effectively deliver drugs through the dendrimer are one of the most widely studied drug delivery vectors effective. However, large amounts of molecules and large surfaces can cause unexpected side effects and toxic problems in the body. Thus, in this study, the decomposable 1,3,5-triazacetic cores synthesized from amino acids (glucine, valine, cysteine, cerine, aspartic acid, glutamate, etc.) synthesized biodegraders that could be broken down into biologically harmless small molecules in response to the decomposition of polyacryliclate. High flexibility is expected in flexible centers and star-shaped branches. In addition, decomposable cores synthesized from amino acids and breakable ketone branches are expected to reduce cytotoxicity. Spectral analysis characteristics, multiplexed morphology characteristics, in vitro cytotoxicity, and gene silence efficiency are discussed. And we will research pharmacodynamic activity of synthesized materials from amino acids.

Poster Presentation : **ORGN.P-234**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

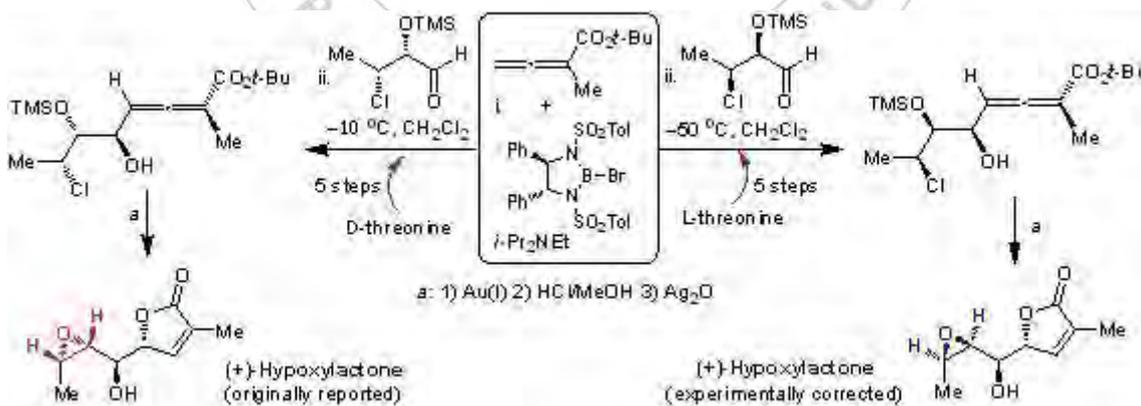
Facile Synthesis of Naturally Occurring (+)-Hypoxylactone through Allenolate Aldol Reaction: Correction of Stereochemical Relationship

Gyungah Pak, Euijin Park, Sehee Yang, Chan-Mo Yu^{1,*}, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

Many organic chemists are attempting to investigate some of these intricate pathways and develop methods to prepare naturally occurring substances in the laboratory. Recently, we developed a highly stereoselective synthesis of unprecedented gamma aldol adducts from the reaction of 2-alkyl allenolates with a chiral bromoborane and base, and then aldehydes. As a synthetic application, we demonstrated an enantiospecific synthesis of (+)-xyloglactone A. We present herein our recent investigations for the synthesis of (+)-hypoxylactone with correction of stereochemistry and clarify a relationship between (+)-hypoxylactone and other butenolides.



Poster Presentation : **ORGN.P-235**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and photochromic reaction of spiropyran-sulfonate containing methoxy group

Eun Ju Shin

Department of Chemistry, Sunchon National University, Korea

Proton-transfer reactions are very important in biological processes and can be used to regulate chemical reactivity, biological functions, and material properties. Photoacid with stronger acidity in the excited state than in the ground state releases a proton upon light irradiation. Photoacid can be used to control protonations and deprotonations. Light as an external trigger can be applied with high precision of location, timing, and dosage. Reversible photoacids can be used in molecular motors and acid-catalyzed reactions. In recent years, spiropyran-sulfonate photoacid attracts great interest for the pH-responsive light-controlled proton transfer reaction. We report preparation of a sulfonate-functionalized protonated merocyanine with methoxy substituent and its reversible protonation and deprotonation 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-236**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and Spectroscopic Properties of Spiropyran-Anthracene Dyad

Hyeji Kim, Eun Ju Shin^{1,*}

Chemistry, Sunchon National University, Korea

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

Spiropyran is the most widely studied photo-switchable compound. Upon irradiation of UV light to colorless and non-fluorescent spirocyanine having two heterocyclic rings connected by a spiro carbon, spirocarbon-oxygen C-O bond is broken to form the highly conjugated zwitterionic merocyanine with a blue or violet color in solution. The merocyanine form returns to the original spirocarbon form thermally or on exposure to visible light. In this study, a new spirocyanine derivative containing anthracene ring, Spiropyran-Anthracene dyad, was designed and synthesized. Spectroscopic properties and photochromic reaction of Spiropyran-Anthracene dyad has been investigated by using ultraviolet-visible absorption and fluorescence spectroscopy.

Poster Presentation : **ORGN.P-237**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and Colorimetric Metal Cation Detection of Rhodamine-thiophene

Bumhee Park, Eun Ju Shin^{1,*}

Chemistry, Sunchon National University, Korea

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

The development of selective optical receptors for the detection of environmentally and biologically important metals has received much attention. Rhodamine exerts excellent photophysical properties such as long absorption and emission wavelengths, high molar extinction coefficient values and high emission quantum yield. Rhodamine is an optical colorimetric sensing probe suitable for the d-block metal cations. We report here a new rhodamine-based colorimetric/fluorometric sensing probe for the selective detection of metal cation. A rhodamine derivative with thiophene substituent has been prepared and characterized by IR, ¹H NMR, and ¹³C NMR spectra. Its metal cation sensing ability has been investigated based on the absorption and fluorescence spectroscopic measurements.

Poster Presentation : **ORGN.P-238**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and photophysical properties of spiropyran-sulfonate containing nitro group

Eun Ju Shin

Department of Chemistry, Sunchon National University, Korea

A spiropyran is a organic photochromic compound and is widely used in medical and technological areas. Photochromic, thermochromic, solvatochromic and electrochromic characteristics of spiropyrans make them especially important in the technology area. Most of their applications are based on their photochromic properties. Irradiation of colorless spiropyran in solution with UV light of wavelength 250–380 nm breaks C-O bonds of spiro ring and generates colored open-ring isomer merocyanine. Because of the apparent conjugated system formed after UV illumination, the extinction coefficient of the open-ring merocyanine form is significantly higher than the one of the closed-ring spiropyran form. Once the irradiation has stopped, the colored merocyanine in solution starts to discolour and to revert to its original colorless spiropyran. Depending on substituent in the aromatic system, the switching behaviour of the spiropyran derivatives can change in their switching velocity and photo-fatigue resistance. In this study, spiropyran-sulfonate containing nitro group has been prepared and its reversible 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-239**

Organic Chemistry

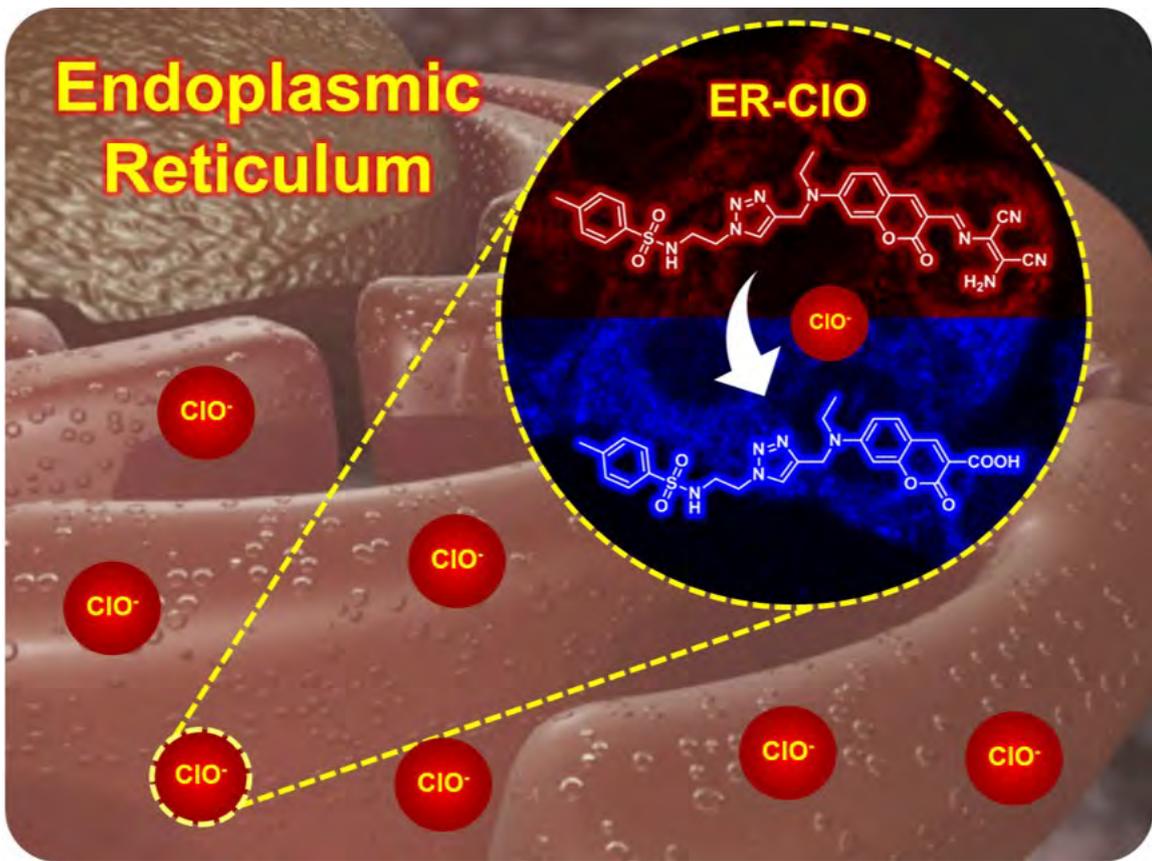
Exhibition Hall 2, THU 11:00~12:30

Coumarin-decorated Schiff base as a ratiometric fluorescent probe for monitoring hypochlorite in Endoplasmic Reticulum

Hyeong seok Kim, Jusung Ahn, Jinwoo Shin, Subin Son, Jiseon Kim, Myung Sun Ji, Ji Hyeon Kim, Wonseok Choi, Inseob Shim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Endoplasmic reticulum (ER), one of the largest cellular organelle, is responsible for the synthesis, folding, modification, and delivery of proteins. ER stress induces an unfolded protein response (UPR) in ER, and mediates complicated signaling pathways, resulting that its increased level is associated with heart diseases, stroke, neurodegenerative disorders, and cancer. Although reactive oxygen species (ROS) have been identified to play a critical role in UPR due to their strong oxidabilities, the exact association of between ROS and ER activity has not been sufficiently revealed yet because of the lack of reliable techniques. Therefore, we have developed a colorimetric and fluorescent probe ER-CIO for the detection of ER ClO^- in a ratiometric manner. This probe rapidly responded to ClO^- with good sensitivity and excellent selectivity. By virtue of the methyl sulfonamide group, the probe was able to accumulate in ER and was successfully applied in the fluorescence imaging of the exogenous and endogenous ClO^- in ER. Owing to its desirable properties, ER-CIO could aid as an efficient tool in the bio-analysis of disease-associated ClO^- variation in ER, which could be useful in various biological and clinical applications, and further research is undergoing.



Poster Presentation : **ORGN.P-240**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Enantioselective [4+1]-Cycloannulation of ortho-Quinone Methides with Diazoesters.

Seungtae Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Chiral 2,3-dihydrobenzofuran derivatives are basic structure of numerous naturally occurring biological active compounds. Although various catalytic methods have been developed, access to chiral 2,3-dihydrobenzofuran through [4+1]-cycloannulation was not fully studied. In this research, we developed the enantioselective synthesis of 2-substituted-3,3-disubstituted-2,3-dihydrobenzofuran catalyzed by chiral oxazaborolidinium ion(COBI) from ortho-Quinone methides and α -alkyl diazoester via tandem Michael-initiated ring closure/intramolecular ring expansion reaction. Various 2,3-dihydrobenzofuran possessing chiral 3-quaternary carbon center were obtained in high yield (up to 94%) with excellent enantio- and diastereoselectivity (up to >99% ee and up to > 20:1 dr).

Poster Presentation : **ORGN.P-241**

Organic Chemistry

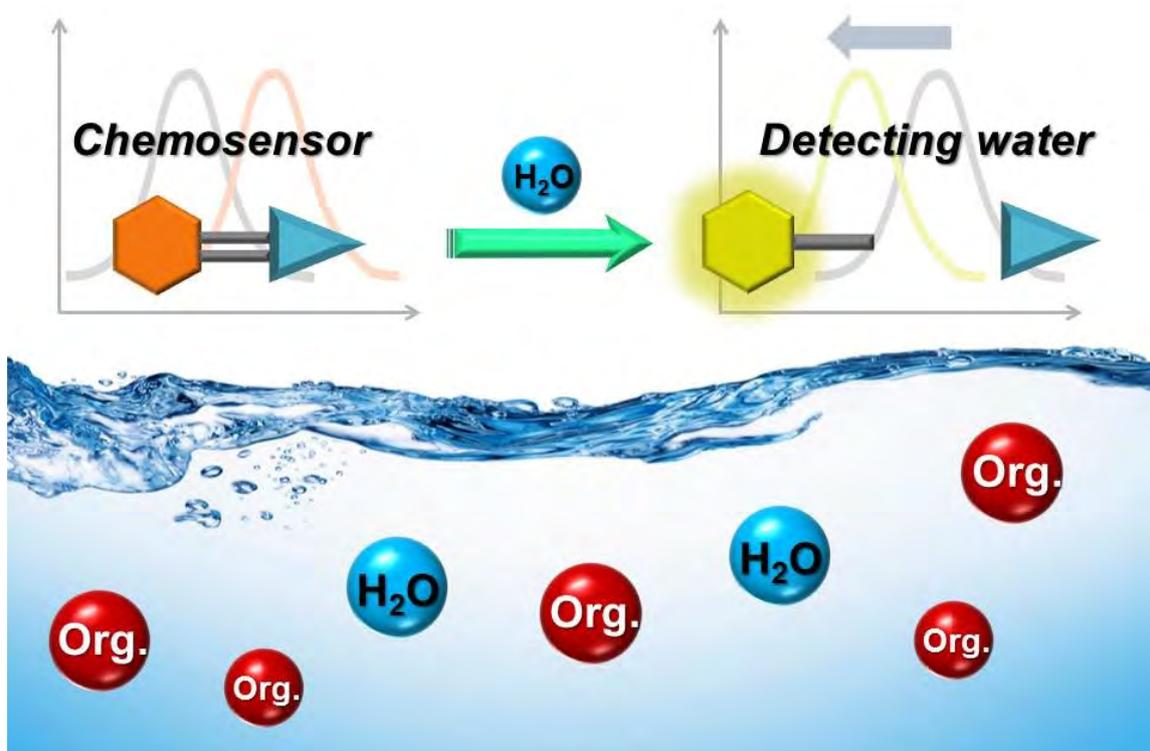
Exhibition Hall 2, THU 11:00~12:30

Coumarin-based Fluorescent sensor triggered by Schiff Base Hydrolysis for the Sensitive Detection of H₂O in Organic Solvents

Jusung Ahn, Hyeong Seok Kim, Jinwoo Shin, Inseob Shim, Subin Son, Jiseon Kim, Ji Hyeon Kim, Myung Sun Ji, Wonseok Choi, Jongseung Kim*

Department of Chemistry, Korea University, Korea

A Chemodosimeter based water sensor was designed and developed for the detection of water in organic solvents. The coumarin-based fluorescent sensor triggered by Schiff base was found to be a sensitive indicator of moisture, via rapid in situ hydrolysis. It showed the prompt optical change upon hydrolysis with H₂O. And also, a structure-relationship examination of a small library of Schiff bases revealed the critical importance of hydrogen bond acceptors in close proximity to the imine bond, and this observation was further supported by theoretical calculations as well as the solid state structure analysis. The most sensitive compound demonstrated a limit of detection and quantification of 0.18% and 0.54% v/v water in DMSO, respectively.



Poster Presentation : **ORGN.P-242**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Drug-containing Zirconium Carbide as a Platform for a New Bio-optical Nanoparticle that can Effectively Treat Cancer

**Inseob Shim, Subin Son, Jiseon Kim, Ji Hyeon Kim, Hyeong Seok Kim, Myung Sun Ji,
Jusung Ahn, Jinwoo Shin, Wonseok Choi, Jongseung Kim***

Department of Chemistry, Korea University, Korea

Conventional photothermal therapy (PTT) faces many major tasks, including inefficient tissue penetration, hyperthermia-induced inflammation, induction of growth factors and cytokines, and metabolic reprogramming. Multi-talented nanomedicine offers an interesting opportunity to avoid the above-mentioned restrictions for successful translation of PTT in clinics. As a deep PTT photosensitizer, a photo-control drug delivery system based on zirconium carbide (ZrC) nanosheet has been developed. A new anti-cancer drug SN38-Nif was inserted into the PEGylated ZrC nanosheet. The SN38-Nif drug was released with photogenic and activated by the esterase with which the tumor was compressed. In vitro and in vivo experimental evidence showed the strong anti-cancer effects of integrated ZrC@prodrug biopotonic nanoplatform, aiming at malignant cells and tumor angiogenesis. In the mouse's hepatocellular carcinoma model (HCC), the ZrC@prodrug-biopotonic nanoplatform system almost eliminated the tumor. Our findings have formulated a new strategy for effective treatment of cancer.

Poster Presentation : **ORGN.P-243**

Organic Chemistry

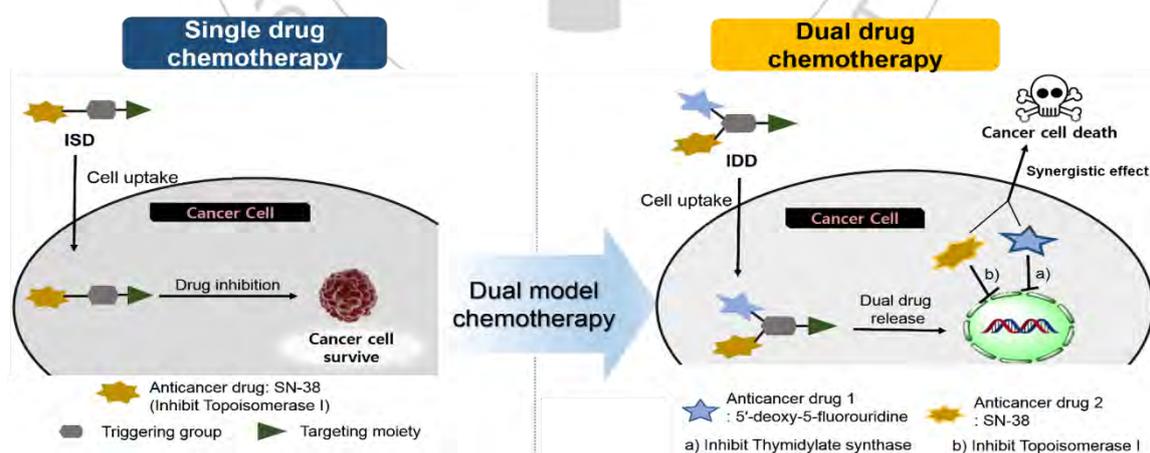
Exhibition Hall 2, THU 11:00~12:30

Binary reinforced first small molecule based COX-2 specific theranostic system for synergistic anti-cancer effect

**Wonseok Choi, Hyeong Seok Kim, Jinwoo Shin, Inseob Shim, Subin Son, Jiseon Kim,
Myung Sun Ji, Ji Hyeon Kim, Jusung Ahn, Jongseung Kim***

Department of Chemistry, Korea University, Korea

We developed an indomethacin-guided, ROS (H₂O₂)-responsive dual drug theranostic probe (IDD) for the cancer selective administration and release of drugs. The comparative In vitro study results of IDD with indomethacin-guided, ROS-responsive single drug theranostic probe (ISD), showed the specificity and efficacy of IDD. IDD and ISD were specifically taken up by COX-2 (+ve) cell lines (MIA-paca-2) over the COX-2 (-ve) cell lines (Caco-2). To our knowledge, this is the first report on small molecule-based prodrug for cancer specific dual chemotherapy system.



Poster Presentation : **ORGN.P-244**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Glycyrrhetic acid-Modified Small Molecular pH Responsive NIR imaging Probe for Hepatocellular Carcinoma (HCC)

**Ji Hyeon Kim, Jinwoo Shin, Hyeong Seok Kim, Inseob Shim, Subin Son, Jiseon Kim,
Myung Sun Ji, Jusung Ahn, Wonseok Choi, Jongseung Kim***

Department of Chemistry, Korea University, Korea

Herein, we reported a glycyrrhetic acid (GA)-decorated small molecule conjugate for pH-triggered near infra-red (NIR) fluorescence imaging of hepatocellular carcinoma (HCC). Our “in vitro” studies demonstrated that NIR-GA was efficiently up-taken by liver cancer cell lines such as HepG2 and Huh7 through GA receptors-mediated endocytic pathway. As suggested by co-localization studies, NIR-GA mainly localized into the lysosome where acidic pH results in activation of fluorescent dye via H⁺-triggered spirolactam ring opening to give strong fluorescence in NIR region.



Poster Presentation : **ORGN.P-245**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Bioorthogonal Two-Photon Fluorescent Probe for tracking a mitochondrial nitroxyl formation

**Jiseon Kim, Myung Sun Ji, Ji Hyeon Kim, Jinwoo Shin, Inseob Shim, Wonseok Choi,
Jusung Ahn, Subin Son, Jongseung Kim***

Department of Chemistry, Korea University, Korea

A bioreductant-resistant 'turn-on' chemodosimetric fluorescent probe Mito-1 has been synthesized for the detection of mitochondrial HNO in live cells. Mito-1 can detect nitroxyl(HNO) as low as ~ 18 nM in live cells. It has the capability to detect not only exogenous but also endogenous mitochondrial HNO formations in cellular milieus demonstrating fluorescence images. Its two-photon imaging ability fosters its use as a noninvasive imaging tool for the detection of mitochondrial nitroxyl.



Poster Presentation : **ORGN.P-246**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Detection of the over-expressing NQO1 levels in cancer using chemiluminescent probe.

**Subin Son, Hyeong Seok Kim, Jinwoo Shin, Inseob Shim, Myung Sun Ji, Jusung Ahn,
Wonseok Choi, Jongseung Kim***

Department of Chemistry, Korea University, Korea

Activatable (turn-on) probes that permit the rapid, sensitive, selective, and accurate identification of cancer-associated biomarkers can help drive advances in cancer research. Here we report a smart novel NAD(P)H:quinone oxidoreductase-1 (NQO1) specific chemiluminescent Probe 1 that allows the differentiation between cancer subtypes. Probe 1 incorporates an NQO1-specific trimethyl-locked quinone trigger moiety covalently tethered to a phenoxy-dioxetane moiety through a para-aminobenzyl alcohol linker. Bioreduction of the quinone to the corresponding hydroquinone initiates a series of steps, which result in a chemiluminescent signal. As inferred from a combination of in vitro cell culture analyses and in vivo mice studies, the probe is safe, cell permeable, and capable of producing a 'turn on' luminescence response in an NQO1-positive A549 lung cancer model. No such signal output was observed in an NQO1-negative H596 lung cancer model. On this basis we suggest that Probe 1 can be used to identify cancerous cells and tissues characterized by elevated NQO1 levels.

Poster Presentation : **ORGN.P-247**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Characterization of Structurally Different Pyrazine Derivatives and Investigation of Their Optical and Electrochemical Properties for Optoelectronic Applications

Dong Jin Park, Sun Hwa Jung, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Pyrazine is an important molecular scaffold employed in organic optoelectronic materials. Here we describe the synthesis and optoelectronic characterization of pyrazine derivatives decorated with donor and acceptor moieties. Using microwave synthetic method has been developed for the preparation of pyrazine derivatives by employing palladium catalysed suzuki coupling reactions. It is identified, if pyrazine derivatives have same functional groups but different structures, they have different optical and electrochemical properties. A comprehensive study of the optical properties, and molecular packing of the synthesized compounds was carried out. The optical and electrochemical properties of the materials are analysed and the results are supported with the DFT calculations.

Poster Presentation : **ORGN.P-248**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Derivatization of dopamine molecules for poly(dopamine) applications

Sangdon Choi, JeongWoo Hong, Yeonwoo Jeong, Sung Min Kang*, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Dopamine is catecholamines, and one of the important neurotransmitter in our nerve system. Not only the biological activities in nervous system, but the role in the organic and surface chemistry is also important. The oxidation of catechol and cyclization promotes the self-polymerization to form thin, surface-adherent polydopamine films onto a wide range of inorganic and organic materials.

In this presentation, we will discuss our recent efforts to synthesize and derivatizing dopamine molecules. We have focused on the aliphatic amine part on dopamine molecules. The carbon chain length was elongated to three-carbons from two-carbons. In addition, the terminal amino group was changed to thiol group to study the functional group effect. The detail synthetic procedures along with characterization will be discussed.

Poster Presentation : **ORGN.P-249**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Photodeprotection for Second Trigger of Poly(dopamine) Coating

Ahrom You, Yeonwoo Jeong, Sung Min Kang*, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Dopamine is simple organic molecule, which is consisting of catechol and aliphatic amines. Dopamine is obtained by removing a carboxyl group from L-DOPA which is synthesized from our brain and kidney. Dopamine is a neurotransmitter. It is released by neuron cell and transfer the neuro signal to other neuron. Dopamine is widely used for not only above biological roles but also surface chemistry. Dopamine has universal coating property with polymerization to poly(dopamine). Oxidation of catechol part to 1,2-hydroquinone and following cyclization is the main reaction for polymerization of dopamine. The oxidation could be promoted in the basic condition and with external oxidant.

In this presentation, the second trigger for dopamine polymerization will be discussed. We have successfully protected catechol functionality with photo-removable protecting groups, and this protected dopamine was applied to the surface coating. The timing of polymerization, even under the oxidative condition, is controlled by UV-irradiation. The detail synthetic procedures along with characterization data will be presented.

Poster Presentation : **ORGN.P-250**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Europium Catalysis: $\text{Eu}^{2+}/\text{Eu}^{3+}$ -based Aerobic Oxidation of Alcohol

Seongwoo Kim, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Europium (Eu) is rare-earth metal, and key element for electronic display devices. The study of europium is generally focused on their photophysical and photochemical properties, and there are very limited reports about catalytic applications of europium.¹ Unlike other lanthanides, europium can have relatively stable two oxidation states (Eu^{2+} and Eu^{3+}) due to the half-filled electronic configuration on f orbital ($4f^7$). Therefore, the redox cycle of $\text{Eu}^{2+}/\text{Eu}^{3+}$ could be utilized in the organic transformation.

In this presentation, our recent study about the europium-catalyzed aerobic oxidation of alcohols to the corresponding aldehydes and ketones will be discussed.² The redox cycle of $\text{Eu}^{2+}/\text{Eu}^{3+}$ was perfectly matched with the oxidation cycle of TEMPO and nitrates, and it successfully applied to the aerobic oxidation of alcohols. The substrate scopes along with the suggestion for mechanism will be presented.

Reference

1. Armelao, L.; Quici, S.; Barigelletti, F.; Accorsi, G.; Bottaro, G.; Cavazzini M.; and Tondello, E. *Coord. Chem. Rev.* **2010**, 254, 487.
2. Kim, S.; Kim, Y.; Jin, H.; Park, M.-H.; Kim, Y.; Lee K.-M.; and Kim, M. *Adv. Synth. Catal.* **2019**, Early View

Poster Presentation : **ORGN.P-251**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of General Synthetic Route for Aspidosperma Alkaloids

Eunjoon Park, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Aspidosperma alkaloids was isolated from old plants of the *Catharanthus roseus*. These alkaloids, which include more than 250 unique members, exhibit significant biological activities. In addition to the biological activities, the unique structure of this class of natural products, bearing a common pentacyclic skeleton, sparked interest within the synthetic community for many years and has remained a focus of immense research activities to date. Structurally, the aspidosperma system is formed by the bond of the C2 of tryptamine with C9 of the secologanin fragment, and it is classified into various characterized structures according to the connectivity. Due to their structural diversity, aspidosperma alkaloids have been synthesized through individual synthesis routes of each natural product. Recently, our group developed a new method for the synthesis of 2-substituted indole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction.¹ With this protocol in hand, all carbon skeletons of Aspidosperma alkaloids could be constructed in the imino-Stetter reaction of aldimine from 2-aminocinnamic acid derivatives and vinyl aldehyde bearing a piperidine ring. The desired natural products can be synthesized by subsequent transformations of the resulting indole product leading to the completion of the total synthesis in very short steps. In this poster presentation, we will describe the racemic and enantioselective total synthesis of goniomitine and our synthetic effort toward aspidospermidine and quebrachamine. Reference 1. Cheon, C.-H. et al. *Adv. Synth. Catal.* 2016, 358, 1566; Cheon, C.-H. et al. *J. Org. Chem.* 2016, 81, 7917.

Poster Presentation : **ORGN.P-252**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of a Synthetic Protocol for 2-Arylquinolines via Palladium-Catalyzed Cascade Reactions

Jooyeon Yoon, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Quinolines are widely found in natural products and pharmaceuticals. Among them, 2-substituted quinolones are particularly important since there are associated with a wide range of biological activities including antimalarial and antitumor activities, as well as being used as a key building block in materials science. Even though numerous methods for the transition metal-catalyzed construction of the quinoline ring system have been reported, there have been few protocols for the synthesis of the simplest 2-substituted quinolones via transition metal-catalyzed cascade reaction. Herein, we report an efficient synthetic method of 2-substituted quinolines from 2-iodoanilines and β -chloropropiophenones, the synthetic equivalents of acrylophenones, in the presence of palladium catalyst. The desired quinolones might be synthesized from these enolate intermediates via two possible reaction pathways. To begin with, oxidative addition of 2-iodoanilines with palladium(0) followed by migratory insertion of acrylophenones would provide palladium(II) enolate intermediates. Subsequent condensation between the amino and carbonyl groups lead the cyclized intermediates. β -hydride elimination of cyclized intermediates would provide the quinoline products. Alternatively, 2-aminochalcones, generated by β -hydride elimination from palladium(II) enolate intermediates, could be converted into the desired quinoline via palladium-catalyzed dehydrative cyclization.

Poster Presentation : **ORGN.P-253**
Organic Chemistry
Exhibition Hall 2, THU 11:00~12:30

Concise Total Synthesis of Phenanthroindolizidine Alkaloids

Young-In Jo, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Since phenanthroindolizidine alkaloids exhibit interesting biological activities, they have received increasing attention in the past decades. In addition to their interesting biological activities, since these natural products possess the different number of methoxy groups around the phenanthrene ring, and the nitrogen atom in the indolizidine ring at the different positions, they have been considered synthetically challenging targets and many different synthetic routes have been developed. Despite these synthetic efforts, most previous approaches have been designed for the synthesis of each specific target molecule through an independent synthetic pathway, and there have been no general synthetic approaches to access these natural products. Despite the structural diversity of these natural products, we recognized structural similarity in these natural products. Since core structures in phenanthroindolizidine natural products possess ortho-terphenyl structure, we envisioned that these natural products could be prepared via the iterative Suzuki-Miyaura reaction of ortho-bromophenyl MIDA boronates.[1] Furthermore, the indolizidine structure, including the different positions of the nitrogen atom, could be derived from pyridine scaffolds.[2] In this poster presentation, we will describe the development of a general synthetic route for phenanthroindolizidine alkaloids. Reference 1. Lee, C.-Y.; Cheon, C.-H. *Adv. Synth. Catal.* 2017, 359, 3831. 2. Park, E.; Cheon, C.-H. *Org. Biomol. Chem.* 2017, 15, 10265.

Poster Presentation : **ORGN.P-254**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Novel Synthetic Method for Construction of 3,4'- Biquinolines

Jiye Jeon, Juhyeon Park, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Biquinoline linked by a single bond between two quinoline moieties have attracted a lot of attention from the chemical society due to their various roles as ligand and potentially interesting biological activities. Despite its interesting properties, only a few synthetic protocols for construction of biquinoline scaffold have been reported. Moreover most reported methods exhibited limited substrate scopes. For these reasons, the development of novel strategies for efficient construction of biquinoline structure is still of need. Very recently, our group developed a synthetic protocol for construction of 2-aryl substituted quinoline from 2-aminochalcones catalyzed by a nucleophilic catalyst.^{1,2} The 1,4-addition of the nucleophile to 2-aminochalcone gave the corresponding saturated ketone analogues, which could have a conformation where the amino and carbonyl groups are proximate. Subsequent condensation between the amino and carbonyl groups and elimination of iodide gave the desired 2-aryl substituted quinoline. We hypothesized that when an anion generated from 1,4-addition of a nucleophile undergo Michael addition to another molecule of 2-aminochalcone, the dimerized structure of quinoline could be synthesized. Based on this working hypothesis, when the t-butoxide was used as nucleophile, 3,4'-biquinolines were obtained from 2-aminochalcones. Furthermore 2-aminochalcone derivatives having various functional group could be applicable to this protocol. We also could define the reaction mechanism by control experiments and high resolution mass spectrometry (HRMS). Reference 1. Lee, S. Y.; Jeon, J.; Cheon, C.-H.; J. Org. Chem. 2018, 83, 5177. 2. Lee, S. Y.; Cheon, C.-H.; J. Org. Chem. 2018, 83, 13036.

Poster Presentation : **ORGN.P-255**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

General Strategy for Synthesis of Corynanthe Family via Intramolecular Imino-Stetter Reaction Followed by Functionalization of Pyridine Ring

Cheolwoo Bae, Eunjoon Park, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Corynanthe alkaloids, isolated from old plants of the *Catharanthus roseus*, have unique structure originated from skeleton of the secologanin. These alkaloids are valuable because they have various pharmacological activities. For this reason, many synthetic methods of Corynanthe have been developed over a long time. One of the most common methods to access the core indoloquinolizine structure is C-3 functionalization of imines or amides derived from tryptamine via either Pictet-Spengler reaction or Bischler-Napieralski reaction. However, these methods generally require additional steps to generate the six-membered D-ring. Recently, our group developed the methods to access indole-3-acetic acid derivatives bearing a pyridyl moiety at the 2-position via the cyanide-catalyzed intramolecular imino-Stetter reaction of aldimine obtained from 2-aminocinnamic acid derivatives and various pyridinecarbaldehydes.¹ In this poster presentation, we disclose our efforts via the functionalization of the pyridinium ring of 2-pyridyl indole-3-acetic acid derivatives to construct the piperidine ring present in Corynanthe alkaloids. This approach allowed us to develop a general synthetic protocol toward Corynanthe family. Reference 1. Park, E; Cheon, C.-H. *Org. Biomol. Chem.* 2017, 15, 10265

Poster Presentation : **ORGN.P-256**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Two-photon Absorbing NIR emitting dipolar dye for bioimaging application

Changwook Song, Kyo Han Ahn*

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

Biological process monitoring by fluorescence detection has several advantages such as non-invasiveness, accessibility, safe detection and simple operation with low cost. However, autofluorescence interference from biomolecules and penetration depth limits the use of fluorescence dyes on clinical site. A two-photon absorbing (TPA) dipolar dye that emits in the far-red or NIR region can be a solution to those issues. Therefore, the development of TPA dipolar dyes are highly required. Such dyes allow us to image of tissue at deeper penetration depth with reduced autofluorescence interference.¹We report naphthalene-based hemicyanine dyes, which have significant two-photon absorbing property and also emit in the NIR region.² The new dyes have high quantum yields, good photostability, and are expected to have minimal autofluorescence interference in two-photon imaging of tissue. Synthesis, characterization of photophysical properties, stability toward reactive oxygen species and biothiols, and an application of the dyes will be presented. 1. Zipfel, W. R.; Williams, R. M.; Webb, W. W. *Nat. Biotechnol.* 2003, 21, 1369. 2. Song and co-workers, manuscript under preparation.

Poster Presentation : **ORGN.P-257**

Organic Chemistry

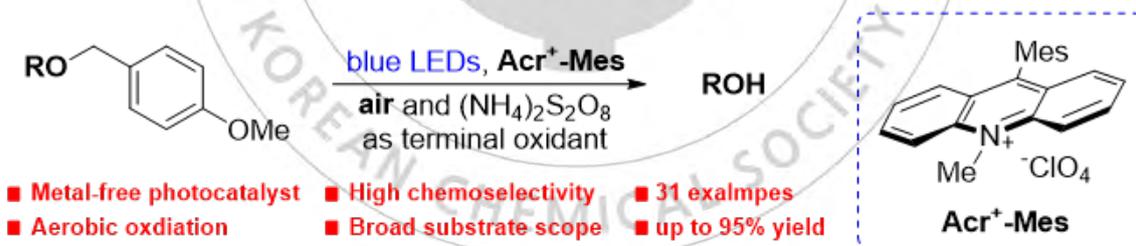
Exhibition Hall 2, THU 11:00~12:30

Visible-Light Photoredox-Catalyzed Oxidative Deprotection of p-Methoxybenzyl Ether

Young Woo Kang, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

An efficient and greener deprotection method for p-methoxybenzyl (PMB) ethers using a metal-free visible light photoredox catalyst and air and ammonium persulfate as the terminal oxidants is presented. Various functional groups and protecting groups were tolerated in the developed method to achieve good to excellent yields in short reaction times. Significantly, the developed method was compatible with PMB ethers derived from primary, secondary, and tertiary alcohols and a gram-scale reaction. Mechanistic studies support a proposed reaction mechanism that involves single electron oxidation of the PMB ether.



Poster Presentation : **ORGN.P-258**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Supramolecular Gels of Fluorescent Aza-Crown Macrocycles: Shape-Dependent Self-Assembly and Size-Selective Response to Ammonium Ion Guests

Suk-il Kang, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Molecular-level host-guest interactions can be amplified to drive macroscopic phase transitions of the bulk material. Using supramolecular gels of π -conjugated macrocycles, we have investigated the effects of guest chemical structures on the gel-to-fluid transition kinetics. While ammonium ions bind only weakly to the individual macrocycles in solution, guest-induced disassembly of gelled macrocycles occur readily under ambient conditions. This net signal amplification process was monitored conveniently by time-dependent UV-vis studies to reveal a straightforward correlation between the response rate and shape/size of the guest species. Well-designed weak links thus respond to subtle differences in weak bonds, and translate them into visually discernible macroscopic signaling events. A proof-of-concept fluorescent turn-on detection system was also devised to demonstrate the practical utility of this design concept.

Poster Presentation : **ORGN.P-259**

Organic Chemistry

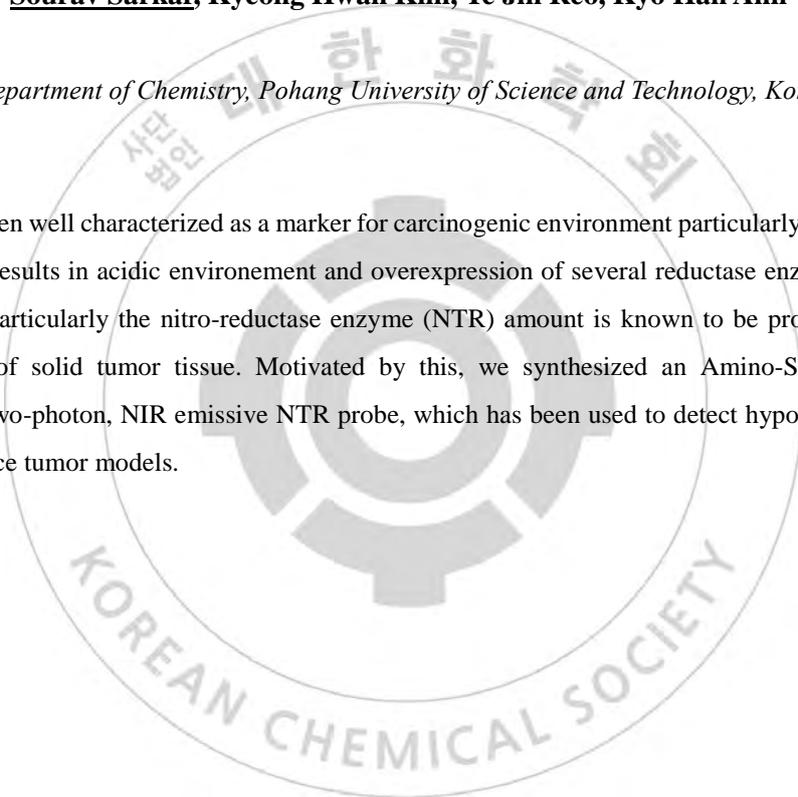
Exhibition Hall 2, THU 11:00~12:30

Amino-Si-pyronin based Ratiometric, Two-photon, NIR emissive probe for monitoring Hypoxia in-vivo

Sourav Sarkar, Kyeong Hwan Kim, Ye Jin Reo, Kyo Han Ahn*

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

Hypoxia has been well characterized as a marker for carcinogenic environment particularly for solid tumor. Hypoxic state results in acidic environment and overexpression of several reductase enzyme inside cell. Among them particularly the nitro-reductase enzyme (NTR) amount is known to be proportional to the hypoxic state of solid tumor tissue. Motivated by this, we synthesized an Amino-Si-pyronin based Ratiometric, Two-photon, NIR emissive NTR probe, which has been used to detect hypoxia state in both cellular and mice tumor models.



Poster Presentation : **ORGN.P-260**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

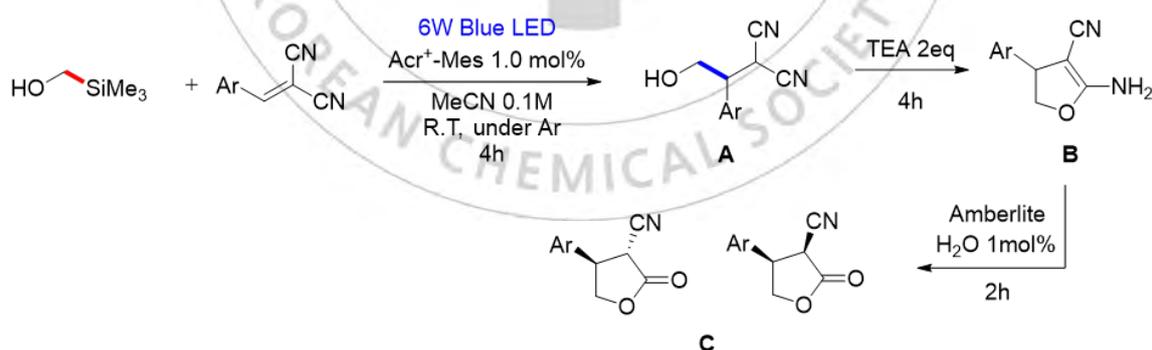
Visible-Light Photoredox-Catalyzed Hydrohydroxymethylation of Activated Alkenes

Subeen Nam, Sang Kook Woo^{1,*}

Chemistry, UNIVERSITY OF ULSAN, Korea

¹Department of Chemistry, University of Ulsan, Korea

Herein, we present a new neutral silicon-based TAG for visible photoredox catalyzed hydrohydroxymethylation of alkenes. This reaction involves in situ generated α -hydroxymethyl radical, useful reaction intermediates in C-C bond forming reactions for functionalization of alcohol, followed by subsequent conjugate addition to activated alkenes. In addition, we can convert to enamine and α -cyano- γ -lactones by cyclization via simple post processing. Various functional groups were tolerated under developed conditions to provide good to excellent yields.



Poster Presentation : **ORGN.P-261**

Organic Chemistry

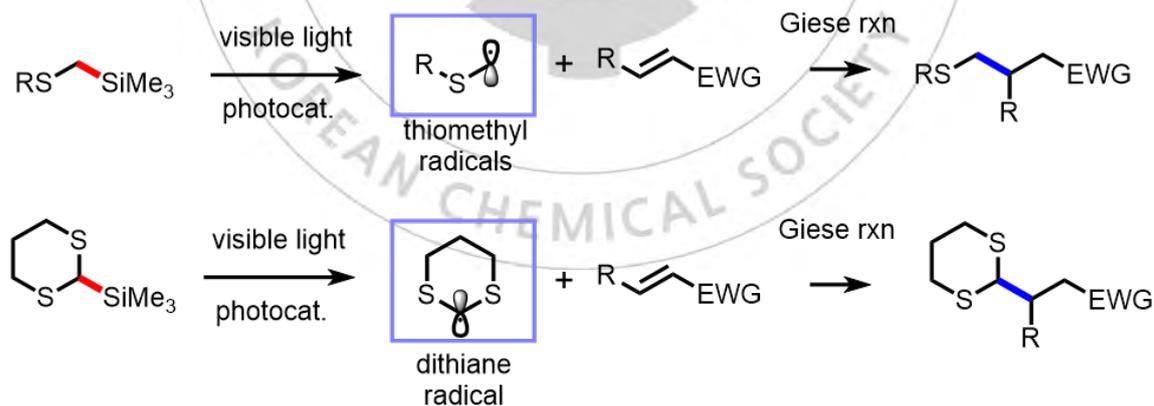
Exhibition Hall 2, THU 11:00~12:30

Photocatalytic Giese Reaction of Methyl Sulfides or Dithianes with Alkenes

Suhyeon Kim, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

Visible-light mediated photoredox catalyzed Giese reaction of methyl sulfides or dithianes with alkenes is described. This reaction involves in situ generated methyl sulfide radicals or dithianes by single electron oxidation of α -TMS substituted sulfides, followed by subsequent conjugate addition to activated alkenes. Various functional groups were tolerated under developed conditions to provide good to excellent yields. Furthermore, the addition products were transformed into valuable synthetic building blocks such as aldehydes, ketones, and alkanes.



Poster Presentation : **ORGN.P-262**

Organic Chemistry

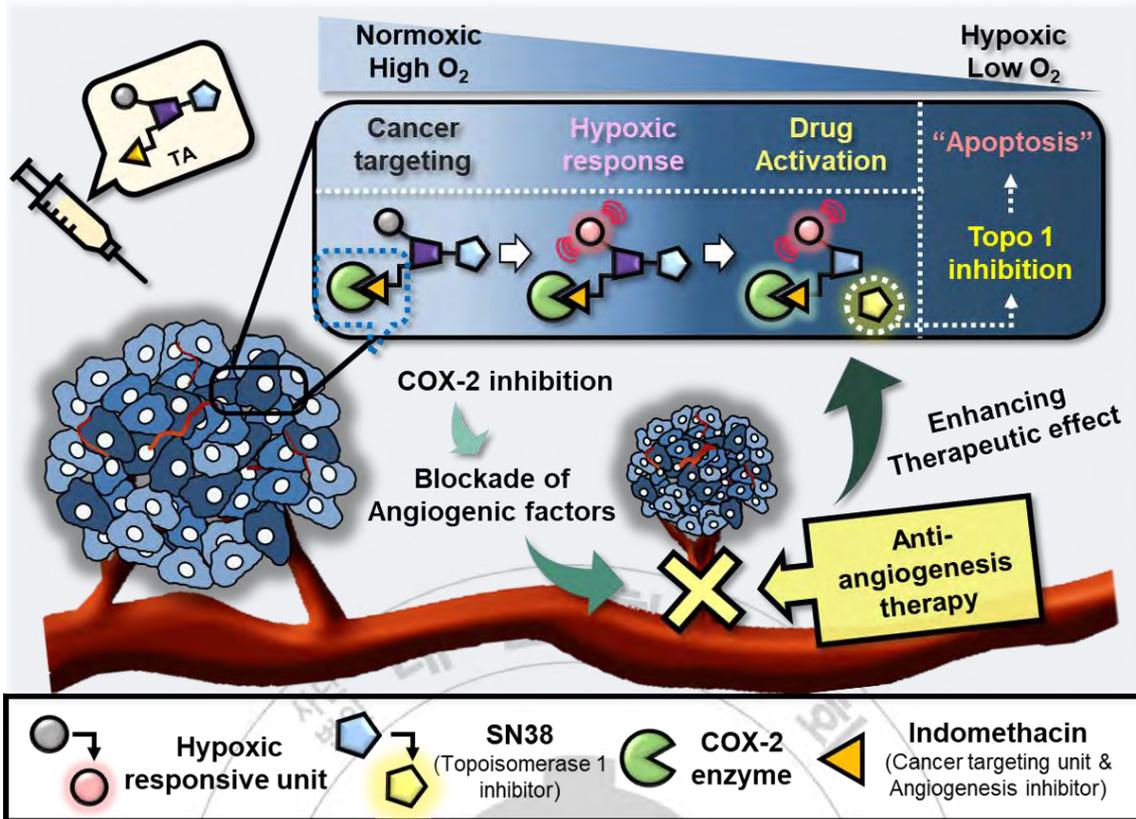
Exhibition Hall 2, THU 11:00~12:30

COX-2 blockade mediated Hypoxia-responsive Anti-angiogenic Prodrug

Eun ji Kim, Hyeong Seok Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

We have developed a novel anticancer DDS for the first time by utilizing indomethacin (IMC) as a COX-2 inhibitor, for an active tumor targeting and angiogenesis inhibition to enhance the therapeutic potential of the hypoxia-responsive prodrug in solid tumors. Unlike traditional approaches for hypoxia triggered DDS carrying active tumor targeting via ligand-receptor interactions, the IMC incorporated TA possesses the capacity to recognize the tumor-associated inflammatory response, such as COX-2 and angiogenesis inhibition (VEGFA, CD31, ANGPT v2, and ANGPT v3) to potentiate the hypoxia in tumor region. The induced hypoxia then significantly potentiates the nitro functionality bio-activation in TA resulting in an active SN-38 release in tumor tissues in a spontaneous and on-demand manner. Likewise, the diagnostic probe DA was developed to image the cancer cells selectively. As a proof of concept, we compared the therapeutic efficacy of TA with reference (R1). Our results demonstrated the remarkable tumor inhibition in TA treated xenograft animal models with no noticeable systematic toxicity. These results showed that concomitant anti-angiogenesis by COX-2 blockade presents an innovative strategy to achieve the synergetic treatment efficacy of hypoxia-responsive prodrugs and foresees possibility to treat patients with metastatic disease in future.



Poster Presentation : **ORGN.P-263**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

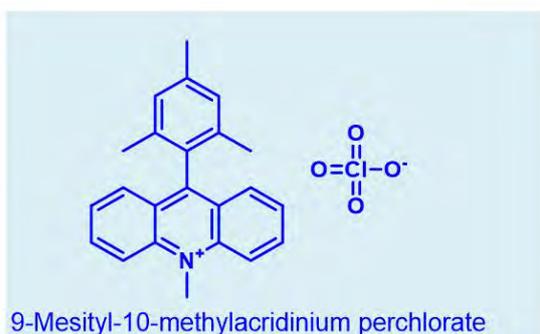
Regioselective allylation of Activated Alkenes using Allylsilanes via Visible Light-mediated Photoredox-catalysis

Arjun Gontala, Sang Kook Woo^{1,*}

Department Of Chemistry, University Of Ulsan, Korea

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

Visible-light mediated photoredox-catalyzed highly regioselective allylation of activated alkenes is described. The reaction involves in situ generated allylic radicals from allylsilanes via photoinduced single electron transfer (SET) mechanism, which subsequently adds regioselectively to the activated alkenes. The reaction features ambient conditions, metal-free condition, with no extra additives, tolerates various photosensitive functional groups and display broad substrate scope. The reaction is also feasible on a gram scale. Allylated products serve as a useful reactive set and undergo diverse synthetic transformations.



- Metal free
- No external additives
- Redox Economical
- Ambient Condition

Poster Presentation : **ORGN.P-264**

Organic Chemistry

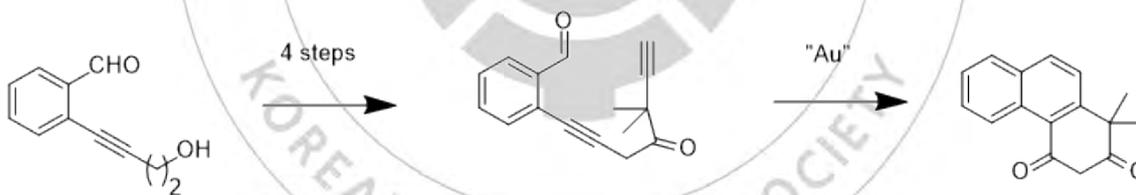
Exhibition Hall 2, THU 11:00~12:30

Synthesis of [6,6,6] abietane system using Au catalyst

Jegeun Jo, Juyeon Kang, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

Abietane structures are often found in nature. Abietane is line of diterpenoids. it is as known as variety of natural chemical compounds such as abietic acid, carnosic acid. Diterpenes are based on compounds such as retinol, retinol and pyrrole. We have initiated to study how to synthesize abietane skeleton. The [6,6,6]-tricyclic could be synthesized as the main product using the diynals like 1. Here we wish to report the synthesis of abietane model structure by using Au catalyst. This reaction was used to study the synthesis of abietane-based natural skeletons.



Poster Presentation : **ORGN.P-265**

Organic Chemistry

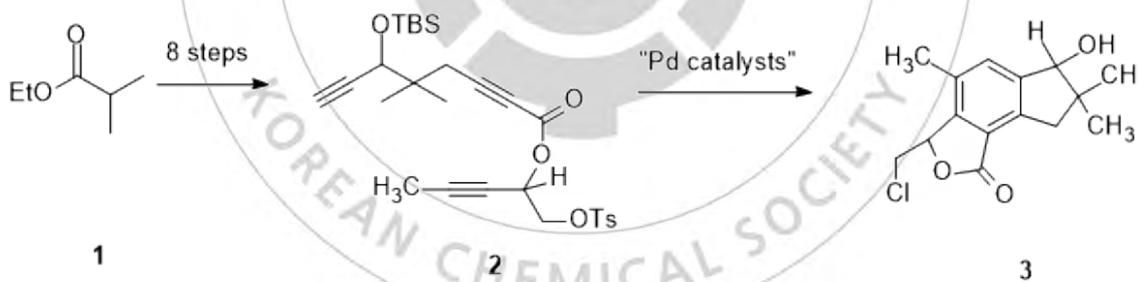
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Alcyopterosin L by using Pd catalyzed-[2+2+2] intramolecular cycloaddition as a Key step

Chaehyeon Seong, Juyeon Kang, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

In modern organic synthesis, the synthesis of natural products having activity is a very important challenge that can physiologically have an effect on the human body. Transition metals are known to act as strong cyclization catalysts. Palladium catalysts, in particular have been known to effectively induce intramolecular cyclization of triynes. We will report among others the synthesis of Alcyopterosin L with by using Pd catalyzed [2 + 2 + 2] intramolecular cycloaddition in 10 steps.



Poster Presentation : **ORGN.P-266**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

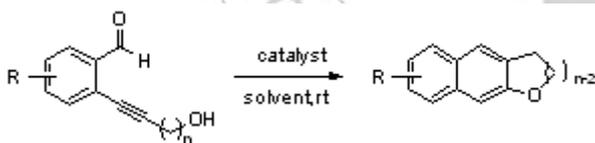
Synthesis of 2,3-Dihydronaphtho[2,3-b]furan by Transition-Metal or Acid-Catalyzed Cyclization

SeungLyeol Lee, Le Thuy Quynh¹, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

¹Chemistry Department, Hanyang University, Korea

We have synthesized 2-(4-hydroxybut-1-yn-1-yl)benzaldehyde by taking advantage of the sonogashira reaction of 2-bromobenzaldehydes with n-alkyn-1-ols. Benzochromanes were obtained from the reaction with ortho-formylarylacetylenols ($n = 4$) when AuCl_3 was employed as the catalyst¹ while the reaction of the aldehyde precursors required a one-pot two-step approach when AgTFA was employed as the catalyst². We have been attempted to find an efficient method leading to the corresponding oxycyclic naphthalenes by utilizing transition-metal or any acid catalysts.



Poster Presentation : **ORGN.P-267**

Organic Chemistry

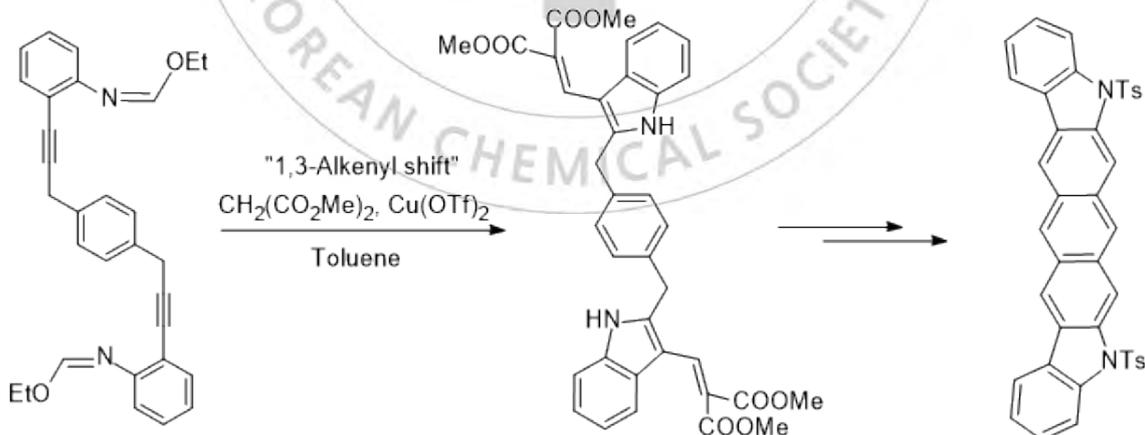
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Polyaromatic Carbazole via 1,3-Alkenyl Shift of N-Arylformimidates

Chang Ho Oh*, **Uiseong Chai**

*Department of Chemistry and Center for New Directions in Organic Synthesis, Hanyang University,
Korea*

Application of heteroacene compounds for organic solar cells and organic field effect transistors has been reported owing to their electrochemical properties. As a part of heteroacene, polyaromatic carbazole was synthesized through 1,3-alkenyl shift of two N-arylformimidates in a molecule. 1,3-alkenyl shift of one site has been reported and adapting to two or more sites at once can be challenged. Thus, we synthesized the polyaromatic carbazoles. The improvement of reaction conditions of 1,3-alkenyl shift was expected to apply for synthesis of polycyclic carbazoles.



Poster Presentation : **ORGN.P-268**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design, synthesis, Acetylcholinesterase inhibitory activity and Molecular docking analysis of 1,2,4-triazolidine-3-thiones

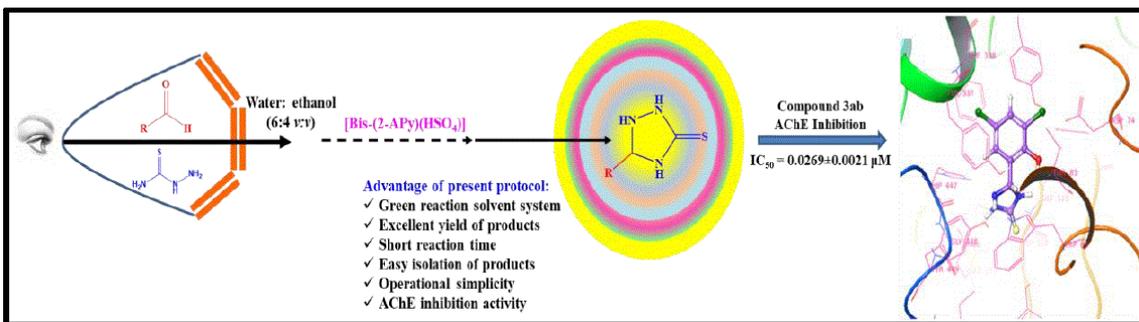
Prasad Gajanan Mahajan, Nilam Chandrakant Dige¹, Balasaheb Daniyal Vanjare, Seong-Karp Hong², Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

¹*Department of Biological Sciences, Room No. 303, College of Natural Science (Building No. 11), Kongju National University, Gongju, Chungnam 32588, Re, Korea*

²*Department of Biomedical Engineering, Mokwon University, Korea*

Triazole derivatives are one of the important compounds in heterocyclic chemistry due to their wide pharmaceutical utility. Triazoles were classified according to the position of nitrogen atoms in the ring viz. 1,2,3- and 1,2,4-triazoles. Amongst which, 1,2,4-triazoles bearing thione moiety exhibit range of biological activities. Hence synthesis of 1,2,4-triazole-thione derivatives is the main motivation of scientist working in the organic chemistry. Herein, we have design and synthesize a novel acidic ionic liquid (IL) and explore its catalytic efficiency in the synthesis of 1,2,4-triazolidine-3-thiones derivatives using simple reaction of substituted aldehydes, salicylaldehydes and heterocyclic aldehydes with thiosemicarbazide in 60:40 v/v water: ethanol solvent system at ambient temperature in shorter reaction time. The formation of target compounds confirmed by NMR, IR and Mass analysis. Pleasingly, some of synthesized compounds shows noteworthy inhibitory activity against acetylcholinesterase (AChE) enzyme with much lower IC₅₀ value than standard Neostigmine methylsulfate. References: 1.S. Maddila, R. Pagadala, S. B. Jonnalagadda, Lett. Org. Chem. 2019; 10:693–714.2.M. Amir, S. Kumar, Acta Pharm. 2007; 57:31-45.3.R. Ramesh, A. Lalitha, RSC Adv. 2015; 5:51188-51192.



Poster Presentation : **ORGN.P-269**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Rhodamine derivatives as potent urease inhibitors: Design, Synthesis, biological estimation and molecular docking analysis

Balasaheb Daniyal Vanjare, Prasad Gajanan Mahajan, Nilam Chandrakant Dige¹, Ki Hwan Lee*

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In this work, a series of the rhodamine 6G based derivatives 5(a-g) were synthesised and assessed for in-vitro urease inhibition and in-silico molecular docking. The synthesis of the heading compounds originated by the esterification reaction of the different acid derivatives 1(a-g), followed by hydrazide formation 3(a-g). Here, rhodamine 6G an electrophile finally coupled in presence of the potassium tert-Butoxide with different hydrazide derivatives 3 (a-g) to form the targeted N-(3', 6'-bis (ethyl amino)-2', 7'-dimethyl-3-oxospiro [isoindoline-1, 9'-xanthene]-2-yl) benzamides derivatives 5(a-g). The structural interpretation of the synthesised compounds was confirmed by using IR, ¹HNMR, ¹³C-NMR and LC-MS analytical techniques. The synthesized compounds 5(a-g) were explored for the in-vitro screening against the Jack bean urease, the result reveals that all the most compounds shows a potent urease inhibitory activity against this enzyme but among the series the compound 5a with an IC₅₀ value of 0.1108±0.0038 μM shows to be most auspicious inhibitory activity comparative to standard drug (Thiourea) having IC₅₀ value 4.7201±0.0546 μM. Furthermore, the docking studies were used to check the binding interaction between the enzyme and the inhibitor. References: 1) Roberts BP, Miller BR, A. E. Roitberg, Merz KM (2012) Wide open flaps are key to urease activity, J. Am. Chem. Soc., 134:9934–9937. 2) Aslam M, Mahmood S, Shahid M, Saeed A, Iqbal J (2011) Synthesis, biological assay in vitro and molecular docking studies of new Schiff base derivatives as potential urease inhibitors, Eur. J. Med. Chem., 46:5473–5479.



Poster Presentation : **ORGN.P-270**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Facile synthesis and in vitro cytotoxic activity of novel indolinone hydrazides

Muhammad Hanif, Muhammad Rafiq¹, Muhammad Saleem², Ki Hwan Lee^{3,*}

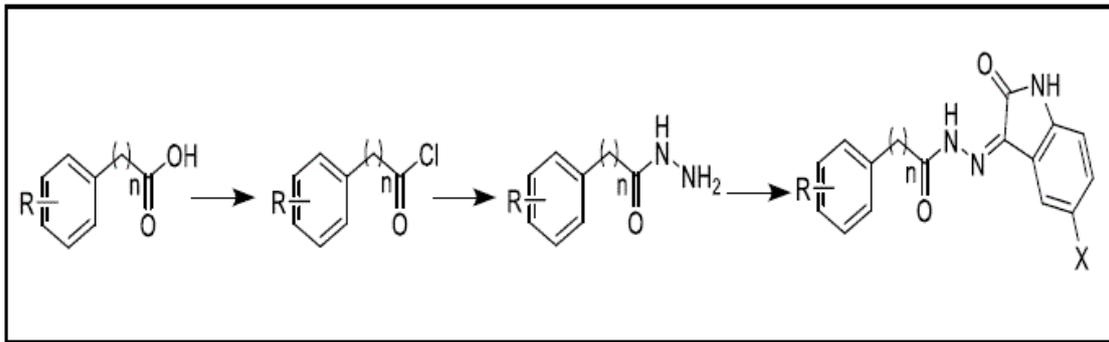
Department of Chemistry, GC University Faisalabad (sub campus layyah), Pakistan

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²*Department of Chemistry, University of Sargodha, Sub-campus Bhakkar, Pakistan*

³*Department of Chemistry, Kongju National University, Korea*

A series of 17 isatin Schiff base derivatives 4a-q were synthesized by refluxing varieties of Haloisatin with the appropriate aralkanoic acid hydrazides 3a-e in order to explore the effect of structure on their bioprofiles. The aralkanoic acid hydrazides 3a-e was synthesized from aralkanoic acid chlorides 2a-e on drop wise addition of the mixture containing hydrazine hydrate and triethylamine in acetonitrile followed by reflux for 3 hr. The synthesized compounds were characterized by the FT-IR, ¹H NMR, ¹³C NMR spectral analysis and evaluated for their cytotoxic activity using three different cell lines including HSF (Human Skin Fibroblast Cells), Hella Cells (Cervical Cancer Cells) and Vero Cells (Kidney Epithelial cells) by using taxol as reference standard. The analogue 4d exhibited maximum cytotoxic activity on Hella cells with percentage inhibition of 81 % at 50 μ M and 100 % at 150 μ M concentrations while 4c showed minimum cytotoxic activity with the value of 21 % at 50 μ M and 23 % at 150 μ M concentrations. References: 1.K. Han, Y. Zhou, F. Liu, Q. Guo, P. Wang, Y. Yang, B. Song, W. Liu, Q. Yao, Y. Teng, P. Yu, Bioorg. Med. Chem. Lett. 2014, 24, 591. 2.G. Chen, Y. Wang, X. Hao, S. Mu, Q. Sun, Chemistry Central Journal 2011, 5, 37.



Poster Presentation : **ORGN.P-271**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Study on the Reactions and Synthesis of 1,2-Benzisothiazol-3-one-1,1-dioxides with Biological Activity

Seung ryul Lee, Do hun Lee¹, Jong Hyun Cho², Dai Il Jung^{1,*}

Dong-A University, Korea

¹*Department of Chemistry, Dong-A University, Korea*

²*Department of Medical Biotechnology, Dong-A 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 modified on the attached benzene ring are particularly desirable. All the types of saccharin derivatives attract extremely intensive attention for the development of novel bioactive and small-molecule medicines. We report the reactions for four types of saccharin(using saccharin, 2-hydroxymethylsaccharin, chloro saccharin, sodium saccharin). Synthesized saccharin derivatives will be executed evaluation of biological activity.

Poster Presentation : **ORGN.P-272**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Development of novel materials with anticancer activity by Niche chemistry

Minhoe Gu, Ju Hyun Song*

Department of Chemistry, Dong-A University, Korea

Bladder cancer is a malignant tumor that develops in the bladder. Bladder cancer occurs for both men and women, and it is the ninth most common cancer in the world. The treatment of bladder cancer is classified into transurethral resection, radical cystectomy, and chemotherapy. Anti-cancer medicine of bladder cancer has highly cell toxicity and can destroy healthy cells causing anorexia, nausea, vomiting, diarrhea, debilitating, and hair loss. Therefore the development of new chemicals that can treat bladder cancer with low side effect is required. Lauric acid has been reported to inhibit the proliferation of breast cancer and endometrial cancer cells. To develop novel anticancer medicines with low side effects and highly biological activity we researched Niche chemistry (esterification and acid condensation). We will use lead compounds including lauric acid with biological activity. In particular some lauric acid-induced compounds showed excellent apoptosis of bladder cancer cell.

Poster Presentation : **ORGN.P-273**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Acid-gated Photoswitchable Diarylethene and study of their fluorescence and photochromic efficiency

Hee ju Son, Bade Thirupaiah¹, Kwang-Hyun Ahn^{2,*}

Applied Chemisty, Kyung Hee University, Korea

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²*Department of Applied Chemistry, Kyung Hee University, Korea*

Photochromic materials have been studied due to their properties which can be controlled reversibly by photoirradiation. They can be used in many application such as optical data storage, sunglasses, inks, and so on. Diarylethenes which are the kind of photochromic materials have high thermal stability and fatigue resistance so that they can be industrialized and mass-produced. In this study, we designed photochromic monomers (Dithio Thiophene BTT, Diphenyl Thiophene BTT) and their oxidation forms (Dithio Thiophene BTTO₂, Diphenyl Thiophene BTTO₂) based on mono BTT which is one of the diarylethenes. The monomers were synthesized by Suzuki reaction and were oxidized by mCPBA in order to synthesize their oxidation forms. In addition, we designed DMABTT which can be photoswitching by acid. DMABTT was synthesized by Suzuki reaction from BTT. Then, we studied photochromic properties including absorption spectra and fluorescence and physical properties including fatigue resistance.

Poster Presentation : **ORGN.P-274**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

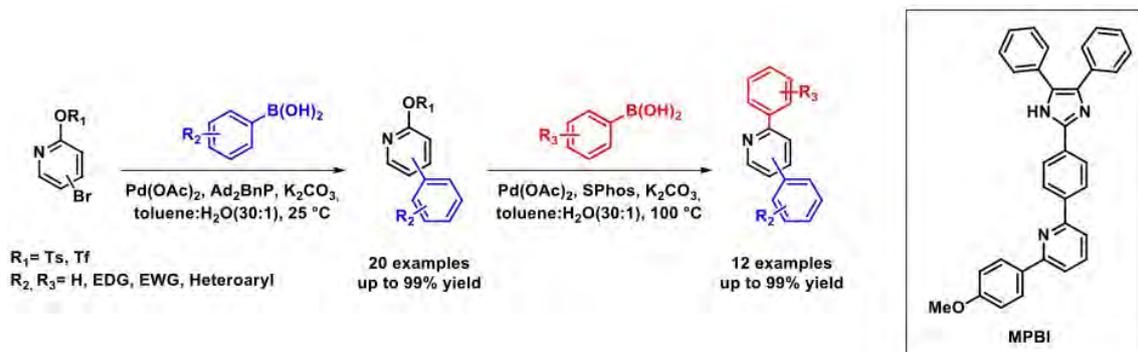
A Synthetic Approach to Unsymmetrical Diaryl Pyridines via Site-selective Suzuki-Miyaura Cross-coupling Reaction

Young-Kyo Jeon, Jae-Yeon Lee, Wonsuk Kim^{1,*}

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

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

Heterocycles containing pyridine are significant units of biologically active synthetic compounds in agrochemical and pharmaceutical fields. Due to their usefulness, lots of synthetic strategies employing transition metal catalysis or organocatalysis to synthesize functionalized pyridines have been reported. However, efficient synthetic methods for the preparation of diaryl pyridines are still necessary. Herein, we present the chemoselective Suzuki-Miyaura coupling reactions for the synthesis of unsymmetrical diaryl pyridines. In general, C2 in pyridine has high reactivity relative to other positions due to its greater electrophilicity. Nevertheless, by using the difference in reactivity between bromo and sulfonyloxy groups, we could successfully suggest chemoselective reaction from bromo-2-sulfonyloxy pyridine. The optimal condition promoted coupling reaction selectively at the bromo group to afford 2, 4, and 6-aryl-tosyloxy or 3-aryltrifloxy pyridines. And further functionalization of the sulfonyloxy group in monoaryl pyridines was accomplished to obtain unsymmetrical diaryl pyridines. In addition, the synthesis of MPBI, a bioactive compound with antibacterial activities, was achieved from 6-bromo-2-hydroxypyridine in 80% overall yield for 3 steps using optimal conditions.



Poster Presentation : **ORGN.P-275**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

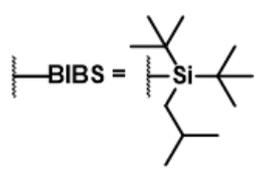
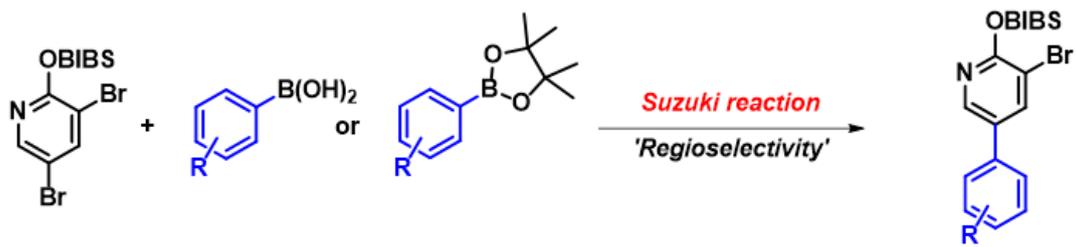
Regioselective Suzuki-Miyaura Coupling of 3,5-Dibromo-2-silyloxy pyridines

Yong-Ju Kwon, Wonsuk Kim^{1,*}

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

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

Regioselective Suzuki-Miyaura coupling reaction on pyridone moiety is valuable in affording diverse bioactive natural products and medicinal compounds. So many different synthetic methods providing aryl substituted pyridone have been developed. Typically, most of them, using C-H activation, radical, and the difference between halogen atoms, presented chemoselectivity on pyridone compound by electronic effect environment. Accordingly, up until now, most strategies has not been deal with steric effect in suggesting chemoselectivity on pyridone structure. Thus, we tried to propose the steric effect in regioselective coupling reaction with utilizing silyl protecting group, di-tert-butylisobutylsilyl (BIBS) group, also easy to eliminate for further application. Depending on the different steric environment of two bromines in starting material, 3,5-dibromo-2-silyloxy pyridine, we could control the rate of the oxidative addition selectively. Herein, we report the regioselective Suzuki-Miyaura cross-coupling reactions for the synthesis of unsymmetrical 3,5-diaryl pyridine derivatives employing 3,5-dibromo-2-silyloxy pyridines with boronic acids and pinacol phenylboronate. Furthermore, one-pot synthesis of unsymmetrical 3,5-diaryl substituted pyridines and the further application synthesis of perampanel, an antiepileptic drug, have been investigated.



R = H, EDG, EWG, Heteroaryl



Poster Presentation : **ORGN.P-276**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

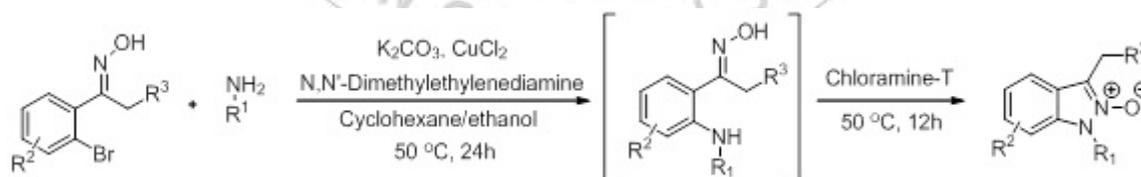
One-pot amination and cyclization of (E)-1-(2-bromophenyl)-ethanone oxime to Indazole N-oxide

JiHyeong Lee, Kyung Hwan Oh¹, Jin Kyoong Park^{1,*}

Chemistry, Pusan National University, Korea

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

Heterocyclic N-oxides are known to have potential biosignificant applications¹. Especially, Indazole N-oxide core performed an important role as an antiprotozoal, antichagasic as well as antiparasitic effect against *T. cruzi* and *Leishmania*². Herein, we have described a facile and efficient synthesis of indazole N-oxide under mild condition. 3-Methyl-1-phenyl-1H-indazole 2-oxide has been synthesized in two steps involving copper-catalyzed amination of (E)-1-(2-bromophenyl)ethanone oxime, followed by cyclization of resulted (E)-1-(2-(phenylamino)phenyl)ethanone oxime using chloramine T as an oxidizing agent. Also, a sequential one-pot synthesis has been investigated to synthesize indazole N-oxide from (E)-1-(2-bromophenyl)ethanone oxime. This method is found to have a wide range of functional group tolerance with moderate to good yields.



Poster Presentation : **ORGN.P-277**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation and characterization of highly soluble acid dyes with high color strength for Digital Textile Printing

Sol Choi, Sang-Yoon Lee, Jun Choi*

Human Convergence Technology Group, Korea Institute of Industrial Technology, Korea

Digital textile printing (DTP) is a process of printing a pattern or image directly designed on a fabric by using an ink-jet injection method. The inks for DTP can be classified into a water-soluble ink and a solvent ink depending on the kinds of fibers used. In this study, we synthesized acid dyes that have high color strength and color purity that can be applied to silk or wool fibers. The perylene, quinacridone and azo structures were used as the moiety of acid dyes and the perylene was finally selected because of its structural stability. The synthesized dyes were designed to have scarlet and high light fastness red. To improve the water solubility of perylene precursors, sulfonic acid groups were introduced at the bay positions of the perylene moiety. In addition, the different functional groups were introduced at the terminal positions of the perylene moiety for improving the light fastness and the optical properties of the dyes. For preparing red acid dyes, we tuned the absorption range by connecting two or four phenol conjugations on the bay positions of the perylene dyes. We found the suitable ink formulation recipes in order to apply the synthesized dyes for high-speed DTP. We analyzed the light and thermal stability of the prepared dyes and compared those properties with the commercial acid dye, acid red 27. The viscosity, conductivity, pH values and color coordinate values of the acid dye inks were measured. The ink jet printing performance of the prepared inks was also investigated.

Poster Presentation : **ORGN.P-278**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Iptycenylic Effects: Stereoelectronic Bias of Bridged Bicyclic Molecular Scaffold to Control Tautomerism and Regioselective Cross-Coupling Reactions

Hongsik Kim, Taewon Kang, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Iptycene chemistry has broad impacts on multiple disciplines in chemistry, including supramolecular self-assembly, crystal engineering, and π -conjugated macromolecules. We recently reported the chemistry of "triazoliptycene", in which 1,2,3-triazole formally replaces one of the three phenyl rings of the iconic triptycene molecule. A last-stage regioselective C–N cross-coupling reaction of triazoliptycene facilitates access to a wide range of fluorescent N2-aryl triazole derivatives having unique photophysical properties. A strong electronic bias toward the N2–H-tautomer, rather than the N1–H-tautomer, of the triazoliptycene is key to the success of this chemistry, which we ascribed to electronically-driven thermodynamic bias to reduce the C–C bond order of the iptycene-fused triazole fragment. The invention (not discovery) of the parent triptycene molecule by Bartlett in the 1940's was motivated by genuine curiosity into the exceptionally stable bridgehead C–X bonds and bond dissociation mechanisms. In this presentation, we will discuss a combined experimental–theoretical investigation to better understand yet another "iptycenylic effect" from the perspectives of electronic structures underpinning the reaction mechanism.

Poster Presentation : **ORGN.P-279**

Organic Chemistry

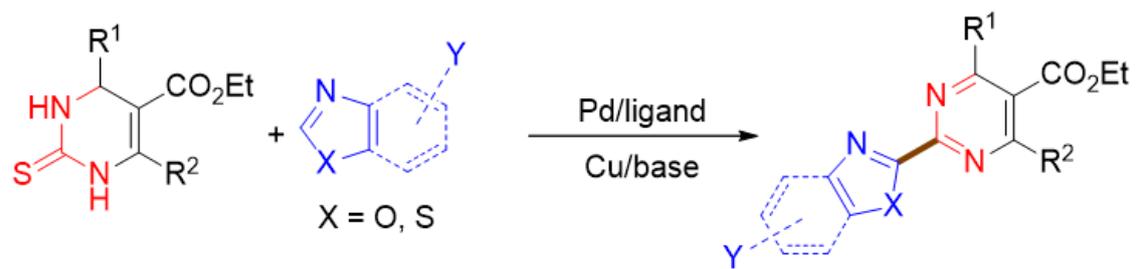
Exhibition Hall 2, THU 11:00~12:30

Synthesis of 2-Azolyipyrimidines via Oxidative Dehydrosulfurative Carbon-Carbon Bond Formation Reaction of 3,4-dihydropyrimidine-1H-2-thiones

Hong Ju Yang, Hyunjoo Kim, Jeong-Hun Sohn*

Department of Chemistry, Chungnam National University, Korea

The pyrimidines were reported to exhibit many pharmacological activities as antimicrobial, antiviral, anticancer, antimycobacterial, anti-inflammatory, antihypertensive, antidiabetic and as inhibitor of xanthin oxidase for treating gout¹. Despite their high importance to these research areas, strategies for synthesizing the various pyrimidine derivatives are limited in terms of their scope and generality with respect to the functionalization of densely substituted varieties. We present dehydrosulfurative C-C cross-coupling reaction of 3,4-dihydropyrimidine-1H-2-thiones (DHPMs) with azoles and concomitant oxidative dehydrogenation under a Pd/Cu catalytic system to provide diverse 2-azolyipyrimidines in a single step.² The reaction proceeded efficiently with a wide range of DHPM substrates and azoles as coupling partners. References 1. (a) Bakavoli, M.; G. Bagherzadeh, M. Vaseghifar, A. Shiri, M. Pordel, M. Mashreghi, (b) P. Pordeli, M. Araghi, *Eur. J. Med.Chem.* **45** **2010** 647–650. (c) N.M. Abunada, H.M. Hassaneen, N.G. Kandile, O.A. Miqdad, *Molecules* **13** **2008** 1501–1517. 2. (a) For oxidative dehydrosulfurative C-N cross-coupling reaction of DHPMs with amines, see: Phan, N. H. T.; Kim, H.; Shin, H.; Lee, H. –S.; Sohn, J. –H. *Org. Lett.* **2016**, *18*, 5154-5157. (b) For oxidative dehydrosulfurative arylation reaction of DHPMs, see: Kim, H.; Phan, N. H. T.; Shin, H. Lee, H. –S.; Sohn, J. –H. *Tetrahedron* **2017**, *73*, 6604-6613. (c) For oxidative dehydrosulfurative C-O cross-coupling reaction of DHPMs with boronic esters, see: Kim, H.; Lee, H.; Shin, H.; Sohn, J. –H. *Org. Lett.* **2018**, *20*, 1961-1965.



Poster Presentation : **ORGN.P-280**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

N-Heterocyclic Carbene Borane Probes for Two-Photon Microscopic imaging of Hypochlorous Acid: Specialized in Endoplasmic Reticulum

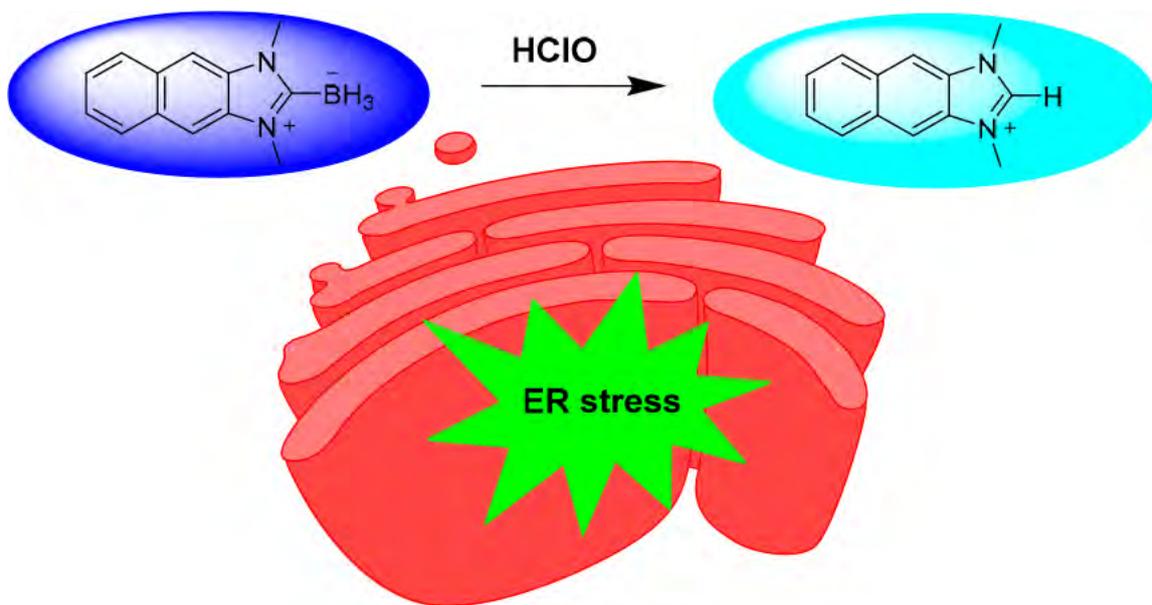
Yubin Yim, Yen Leng Pak¹, Sang Jun Park², Hwan Myung Kim^{2,*}, Juyoung Yoon^{*}

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

¹*School of Chemical Sciences, University of Chinese Academy of Science, China*

²*Department of Energy Systems Research, Ajou University, Korea*

The N-heterocyclic carbene (NHC) borane undergoes oxidative hydrolysis and is an imidazolium salt (ROS) which has superior rate selectivity towards HOCl than other reactive oxygen species (ROS) including peroxides and peroxyxynitrite give. The selectivity for HOCl arises from the electrophilic oxidation mechanism of NHC borane, which is in contrast to the mechanism of nucleophilicization of arylboronic acid by ROS. The change in polarity associated with the conversion of NHC borane to imidazolium salt can control the formation of luminescent excimer and forms the basis for the design of the first fluorescent probe for ROS based on the oxidation of B-H bond .In addition, naphthimidazolium borane 4 has been shown to be a more selective probe for HOCl than other reactive oxygen species. Unlike other boronate-reactive oxygen species (ROS) fluorogenic probes that are oxidized by HOCl via a nucleophilic boronate-dakin oxidation mechanism, probe 4 is cleaved by its electrophilic oxidation mechanism including B-H bond cleavage It is distinguished. Two-photon microscopy experiments on living cells and tissues. Probe 4 is used to monitor endogenous HOCl development and demonstrate changes in HOCl concentration generated in the endoplasmic reticulum during oxidative stress conditions.In addition, two-photon microscopy (TPM) ratiometric imaging of HOCl in living cells and tissues has been demonstrated using each probe



Poster Presentation : **ORGN.P-281**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

In Vivo Albumin Traps Photosensitizer Monomers from Self-Assembled Phthalocyanine Nanovesicles: A Facile and Switchable Theranostic Approach

Nahyun Kwon, Xingshu Li¹, Jian-Dong Huang^{2,*}, Sun Choi^{3,*}, Juyoung Yoon*

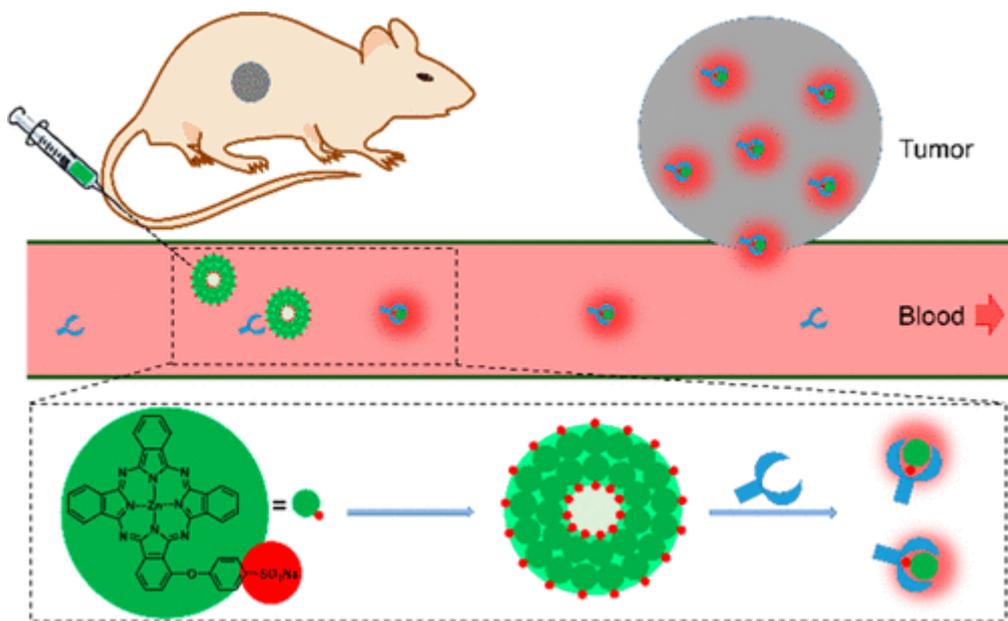
Department of Chemistry and Nano Science, Ewha Womans University, Korea

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Currently, several switchable strategies, such as molecular beacons, aggregation-induced emission, structure-switching aptamers, and supramolecular approaches, have been developed to probe biomarkers and deliver therapeutic agents. Although these theranostic systems permit both diagnosis and treatment by using novel approaches, most of these systems suffer from the requirements of multiple components, extra materials, and multistep fabrication. Therefore, we herein describe a “one-for-all” switchable strategy based on the dynamic assembly- and disassembly-driven nanotheranostics that are constructed using an inherently multifunctional molecule as the building block. In our system, a versatile phthalocyanine derivative bearing a hydrophilic group is designed as the building block. This amphiphilic chemical structure facilitates spontaneous assembly to form a uniform nanovesicle dispersion in aqueous solutions. Interestingly, albumin can trap the phthalocyanine molecule from this nanovesicle and induce its disassembly, leading to switchable photoactivity. Thus, our nanovesicle assembly possesses several highly competitive characteristics: (1) it is self-assembled from one pure component without complex processes; (2) the targeted protein-driven “turn on” fluorescent signal permits the potential application of our nanovesicle assembly for in vivo albumin labeling and tumor imaging with relatively high signal-to-background ratios; (3) the in vivo latent albumin-triggered reactive oxygen species (ROS) generation provides a high possibility for time-modulated, activatable photodynamic therapy (PDT) with minimal side effects.



Poster Presentation : **ORGN.P-282**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Colorimetric and ratiometric detection of mercury using two-photon fluorescent probe

Gain Baek, Liyan Chen¹, Sang Jun Park², Hwan Myung Kim^{2*}, Juyoung Yoon^{*}

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

¹*Department of Chemistry, Central China Normal University, China*

²*Department of Energy Systems Research, Ajou University, Korea*

Selective and sensitive sensing in solutions, living cells and tissues for detecting mercury are in great demand because of its toxicity. We synthesized Naphthalimide-based diphenylphosphinothioyl group-containing colorimetric and fluorescent probe for mercury targeting (Hg²⁺). Upon the addition of mercury to the solution of probe, both a fluorescence change from blue to green (under a 365 nm hand-held UV lamp) and a colorimetric change from colorless to yellow occur that could be observed by “naked-eye”. This probe also has the ability to detect intracellular mercury in both living cells and tissues using two-photon microscopy and dual-emission channels

Poster Presentation : **ORGN.P-283**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

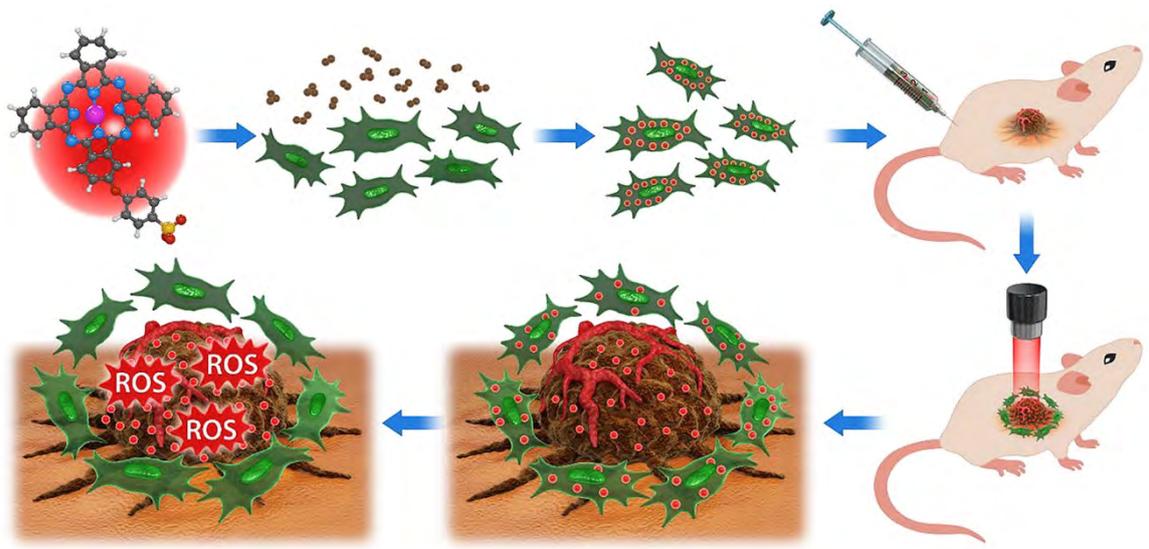
Delivery of Activatable Photosensitizer for Photodynamic Therapy using Human Mesenchymal Stem Cells (MSCs)

Eunhye Lee, Xingshu Li¹, Juyoung Yoon*

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

¹Department of Pharmaceutical Sciences, University of Toronto, Canada

Conventional photodynamic systems rely on passive targeting and active targeting (chemically attached targeting ligands) to provide limited targeting efficiency. Therefore, accurate and selective targeting with minimal side effects is especially important for customized medicine, but it is still a challenge. Here, we present a new approach to the development of precise photodynamic therapy (PDT) using human mesenchymal stem cells (MSCs) to deliver a new activatable photosensitizer (PcS). As a result of real-time optical imaging in vivo, PcS-loaded MSC showed excellent tumor search characteristics. More importantly, it was confirmed that MSCs correctly transfer PcS to human colorectal cancer cells (HCT116) via a "by-stander effect". After local irradiation, the growth of intraperitoneal xenograft tumors was significantly inhibited by photodynamic effects. This discovery represents a promising strategy for accurate photodynamic oncotherapy.



Poster Presentation : **ORGN.P-284**

Organic Chemistry

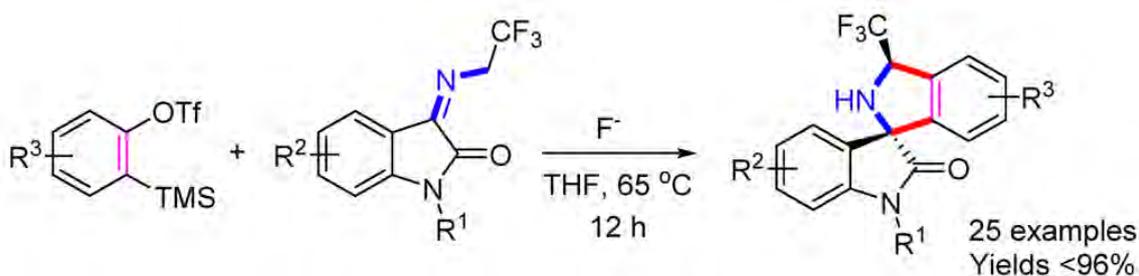
Exhibition Hall 2, THU 11:00~12:30

Synthesis of Spiro[oxindole-3,2'-pyrrolidine] Derivatives from Benzyne and Azomethine Ylides through 1,3-Dipolar Cycloaddition Reactions

Jeongseob Seo, Haye Min Ko*

Department of Bio-nanochemistry, Wonkwang University, Korea

A novel synthetic strategy employing benzyne and azomethine ylides for the construction of spiro[oxindole-3,2'-pyrrolidine] derivatives has been achieved in good yields. The ketimines obtained from the condensation of isatins with $\text{CF}_3\text{CH}_2\text{NH}_2$ react with benzyne in the presence of weak bases such as TBAF or TBAT. This mild practical 1,3-dipolar cycloaddition provides an efficient route to access biologically active compounds.



Poster Presentation : **ORGN.P-285**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Applicable factors for controlling the β -peptide 12/10-helix handedness

Jieun Lee, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

We present the controllable handedness of β -peptide 12/10-helix by adding methyl groups with specific stereochemistry to *cis*-2-aminocyclohexane carboxylic acid(*cis*-ACHC) residues and changing the position of double bond in center residue. Because the helix inversion occurs by ring flipping of the cyclohexane moieties, fixing the conformation of residues can make the oligomer more rigidified. In our laboratory, the first examples of atomic-resolution crystal data for the *cis*-ACHC oligomer with alternating chirality were discovered and in succession, we synthesized oligomers that have small differences in functional groups for comparing folding propensity. First, we synthesized two rigidified pentamers that consist of *cis*-2-amino-*cis*-4-methylcyclohexane carboxylic acid(*cis,cis*-mACHC) or *cis*-2-amino-*trans*-4-methylcyclohexane carboxylic acid(*cis,trans*-mACHC) with cyclohexene and compared them with a pentamer which has no methyl group. From the comparison, we proved that methyl groups affect directions of NH and C=O groups and therefore, they tend to make specific handedness of oligomers in solution. Secondly, we synthesized a pentamer which has a double bond at different position of central residue for probing the effect of double bond position to helical conformation. These controllable handedness of 12/10-helical β -peptide can be a valuable application to foldamer helices.

Poster Presentation : **ORGN.P-286**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Changing folding structure of 12/10-Helical β -Peptides by residue transformation

Yonghan Kim, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

Foldamer refers to a compound capable of forming a certain structure such as a protein found in nature. In the case of oligomers containing β -amino acid, a new form of hydrogen bonding structure that shows a different tendency from alpha was observed. Oligomers containing ACHpC(2-aminocycloheptanecarboxylic acid) has low energy barrier required for interconversion between *M*- and *P*-helix. In order to take advantage of these properties, we are trying to find an oligomer composed of ACHpC which forms a stable skeleton. The 12/10-helical pentamers that consist of *cis*-ACHpC were identified using IR, CD and NMR study. Previous research has shown that the mACHC(2-amino-4-methylcyclohexanecarboxylic acid) can control the N-H binding arrangement to axial or equatorial using the 1,3-diaxial interaction of methyl. This allowed the ring structure and handedness to make up the oligomer were fixed in one direction. We predicted that when introducing the control part in the middle of the pentamers instead of the N-terminus, it is easier to control the helix. Because of β^3 - and β^2 -alanine are expected to be able to control helix by forming *gauche*- conformation in helical structures, we synthesized pentamers containing β^3 - or β^2 -alanine in the middle of the pentamers. We then analyzed the changes in structure and hydrobonding by IR, CD and NMR study.

Poster Presentation : **ORGN.P-287**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

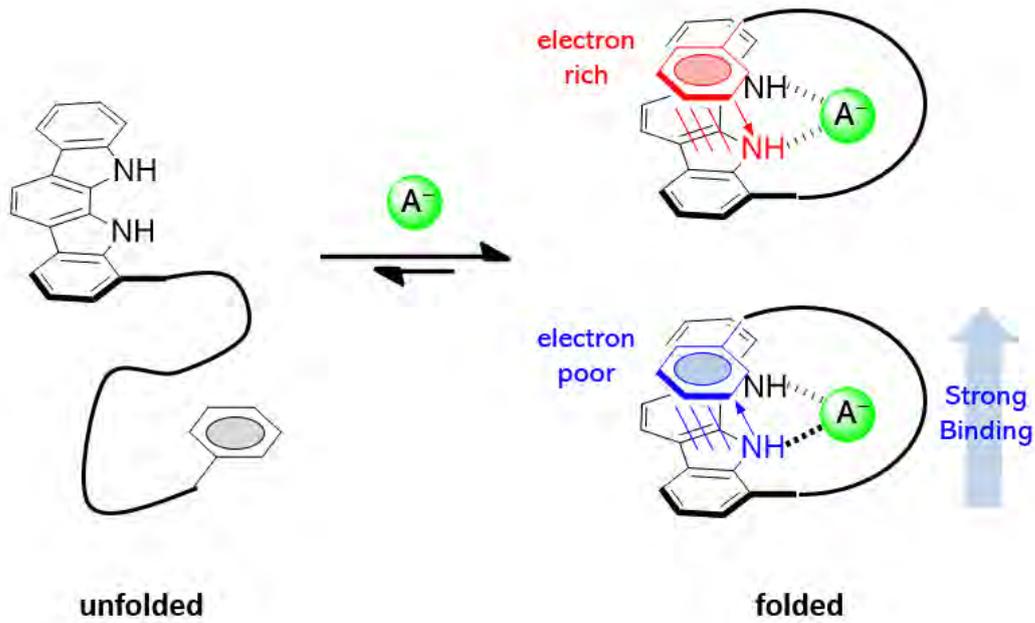
Effects of Aromatic Stacking on the Hydrogen Bonding Interactions between Arylene Ethynylene Oligomers and Anions

Sung Beom Seo, Kyu-Sung Jeong^{1,*}

Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Aromatic hybrid oligomers that consist of Indolocarbazole, pyridine and substituted benzene were prepared and investigated their binding affinities with anions. These oligomers are designed to encapsulate an anion by NH and CH hydrogen bonds, thus folding into a helical structure. All the oligomers have an identical hydrogen bonding moiety but different π -stacking area between aryl planes. Although the aryl appendages at the end of the oligomers does not directly participate in the binding of anions, they have dramatic effects on the magnitudes of the binding affinities; electron-deficient aryl appendages such as pentafluorophenyl greatly increase the association constants between the oligomers and chloride ions. Details will be described in the presentation.



Poster Presentation : **ORGN.P-288**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Allenes through NHC-Cu-catalyzed SN2' Reduction of Propargylic Chlorides with Diisobutylaluminum Hydride

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¹*Department of Chemistry, Kwangwoon University, Korea*

Allenes are important structures existed in natural products and biologically active molecules. Allenes can be also used as valuable intermediates for further synthetic modifications. Therefore, many synthetic methods for synthesis of allenes have been studied. In this study, we have developed an efficient and practical approach to allenes through Cu-catalyzed regio- and stereoselective SN2' reduction of a variety of propargylic chlorides. The propargylic reduction was promoted by the presence of 1-5 mol % of NHC-CuCl catalyst and used readily available and inexpensive DIBAL-H as a hydride source. A new and versatile functionalized allenes were synthesized in good to excellent yields with high regio- and stereoselectivities under mild reaction conditions.

Poster Presentation : **ORGN.P-289**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Porous Organic Solids: Sliding and Breathing Motions through Molecular “Single Point Mutation”

**Taewon Kang, Hongsik Kim, Sungeun Jeung¹, Dohyun Moon^{2,*}, Hoi Ri Moon^{3,*},
Dongwhan Lee***

Division of Chemistry, Seoul National University, Korea

¹*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

²*Beam Operation Team, Pohang Accelerator Laboratory, Korea*

³*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Porous materials have been applied for various purposes including gas storage and separation. One strategy to provide structural and functional adaptability to those materials is introducing stimuli-responsive motifs into rigid network structures such as metal-organic frameworks (MOFs) or covalent organic frameworks (COFs). The network structures typically serve as passive grids that support functional units having desired properties. In this work, we report an inherently different strategy to develop environment-adaptive porous organic solids. By organizing non-stackable X-shaped organic molecules mainly by dispersive C–H \cdots π interactions, we have prepared organic crystals having unobstructed channels. Due to the highly flexible nature of the weak forces that hold non-stacking molecules in the solid-state, the channels spontaneously change their shapes depending on the external environment. Such unique structural properties result in double-step adsorption isotherm and large desorption hysteresis. Comparative studies of isosteric analogs designed by chemical “single point mutation”, in conjunction with in-situ X-ray diffraction analyses, revealed a fine balance of repulsive and dispersive interactions responsible for the observed flexibility.

Poster Presentation : **ORGN.P-290**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Promotion of Hetero Diels-Alder Reaction *via* Intermolecular Hydrogen-bonding

GwangJin Kim, Bongjin Moon*

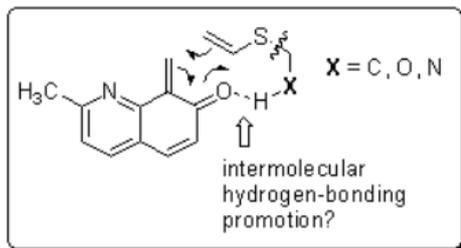
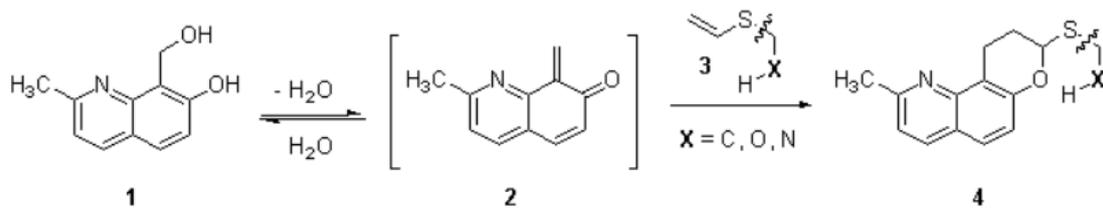
Department of Chemistry, Sogang University, Korea

Ortho-quinone methide can be generated *in situ* by dehydration of ortho-hydroxymethylphenol and is a useful enophile in hetero-Diels-Alder reaction. 8-(Hydroxymethyl)-2-methylquinolin-7-ol (**1**) generates the corresponding ortho-quinone methide **2** in the same manner and the resulting intermediate **2** gradually reacts with vinyl sulfide **3** to provide the hetero-Diels-Alder product **4**.¹ This reaction is useful in bioconjugation because it can be run in water.

In the course of synthesizing various cyclic thioacetal compounds **4**, we realized that the reaction rates of the hetero-Diels-Alder reaction between **2** and **3** are sensitive to the structure of **3**. Careful investigation indicated that the vinyl thioether **3** bearing a substituent that can provide a hydrogen bonding to the ortho-quinone methide exhibit significantly higher reaction rates. In this study, we have investigated the structural effect of **3** in the pericyclic reaction in depth some of results will be discussed.

References

1. Li, Q.; Dong, T.; Liu, X.; Lei, X. *J. Am. Chem. Soc.* **2013**, *135*, 4996-4999.



Poster Presentation : **ORGN.P-291**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Intra-Mitochondrial Polymerization-induced Self-Assembly using Dynamic Disulfide Bond for Anti-Cancer Treatment

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

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

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

The potential use of intracellular polymerization could be new strategy in cancer theranostics. However, the regulation of polymerization has been still challenging due to spatiotemporal control. Unexpected polymerization can cause cellular damage on normal cells, decrease efficiency of intra-mitochondrial polymerization. In this regards, polymerization consisted of reversible bond would be beneficial due to easily decomposable property, reducing side effect. Disulfide bonds are one of dynamic covalent bonds used in the generation of reversible chemical systems. Under slightly basic condition, thiol group are deprotonated to give thiolate which are oxidized to disulfide. The disulfide bond can be decomposed easily into thiolate group under reduced environment. The high concentration and elevated level of ROS provide effective condition to occur polymerization inside mitochondria of cancer cells. However, low concentration and low level of ROS in normal mitochondria might not be sufficient for polymerization occurrence. In cancer cells, the resulting polymer stress mitochondria, leading to generation of ROS. The oxidative agents catalyze production of a larger amount of polymer, which generates more oxidative agent as autocatalytic emergency, leading to dysfunction of mitochondria.

Poster Presentation : **ORGN.P-292**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

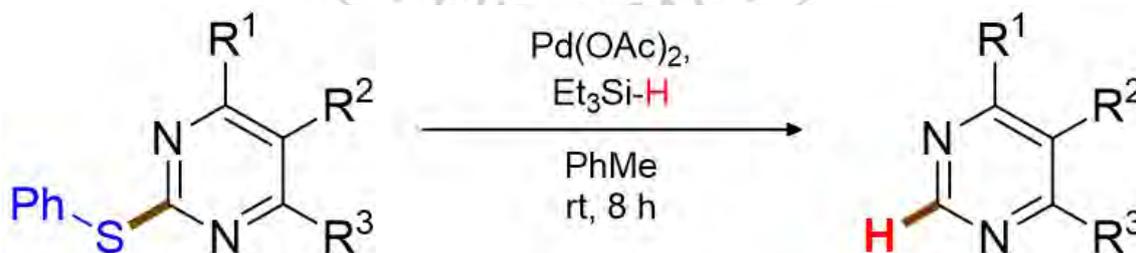
Reductive Cleavage of Thioether for Rapid Access to Pyrimidines substituted at C4-C6 Positions

Yoojin Oh, Jihong Lee¹, Jeong-Hun Sohn^{1,*}

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

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

Pyrimidine structure has attracted much attention from organic and medicinal chemists due to their vast biological profile and thus embedded as a privileged scaffold.¹ Notwithstanding their pharmacological importance by acting as a key binding fragment to the biological targets, synthetic strategies toward the various pyrimidines substituted at C4-C6 positions are restricted in the scope and generality, especially for rapid diversification with regard to the functionalization of the substituted varieties. We report herein the synthesis of the tri-substituted pyrimidines at C4-C6 positions by the reductive cleavage of thioether present at the C2 position of pyrimidines. References 1. (a) Patchett, A. A.; Nargund, R. *P. Annu. Rep. Med. Chem.* **2000**, *35*, 289-318; (b) Lagoja, M. *Chem. Biodivers.* **2005**, *2*, 1-50; (c) *Pharmaceutical Substances: Synthesis, Patents, Applications*; A. Kleemann, J. Engel, Eds.; Thieme: Stuttgart, Germany 2001.



Poster Presentation : **ORGN.P-293**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Temperature-dependent Fluorescence Change of Dye-conjugated Heterotelechelic Poly (2-isopropyl-2-oxazoline)

Ye Ji Kim, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Fluorescence resonance energy transfer (FRET) is an important phenomenon for understanding of some biological systems. FRET is a powerful tool for measuring nanometer scale distances and changes based on the emission. In this research, we synthesized heterotelechelic polymer with tetraphenylethene(TPE) and rhodamine on both ends of poly (2-isopropyl-2-oxazoline) (**T-POx-RM**). To observe the thermo-responsive property of the polymer, the cloud point temperature (T_{CP}) was measured by the transmittance change using UV-Vis spectroscopy. T_{CP} of **T-POx-RM** was determined to be 30°C. FRET is based on the thermo-responsiveness of **POx**. This was confirmed by visual observation and fluorescence measurement. Upon 365 nm UV irradiation, **T-POx-RM** exhibited the blue emission of TPE below the T_{CP} , and above the T_{CP} , **T-POx-RM** exhibited the orange emission of rhodamine. As the temperature increases, the emission intensity ratio of rhodamine to TPE (I_{550}/I_{475}) tends to increase, which increases rapidly around T_{CP} . This system can be used as a thermometer in living organisms.

Poster Presentation : **ORGN.P-294**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of BN-doped naphthalene derivatives with four different substituents

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

Polycyclic aromatic hydrocarbons (PAHs) are conjugated molecules with two or more fused benzene rings. These delocalized pi-electron systems provide the basis of materials for optoelectronic devices, such as OLEDs, OFETs, and OPVs. In particular, their electronic properties can be further tuned if a selected carbon-carbon (CC) bond is replaced by a boron-nitrogen (BN) bond. This CC/BN isosterism would be a powerful strategy to modulate frontier molecular orbitals of target materials. Here, we propose an efficient, modular, and convenient synthetic protocol that allows us to incorporate specific aryl substituents into a BN-doped naphthalene core. In this study, we prepare 2,1-borazonaphthalene derivatives with four different aryl groups by a borylative cyclization reaction and sequential cross-coupling reactions. Overall, we expect that our bottom-up synthesis can be utilized as the way to design new BN-doped materials.

Poster Presentation : **ORGN.P-295**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and electroluminescent properties of 9-(10-phenylanthracen-9-yl)-benzo[b]fluoreno[3,4-d]thiophene derivatives for Blue Organic Light-Emitting Diodes

Soo Kyung Kang, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

Organic light-emitting diodes (OLEDs) have developed rapidly in academic and industrial areas because of potential application. Blue light material has insufficient electroluminescent performances due to the wide energy band gap. In this research, we designed and synthesized four blue emitting materials based on 9-(10-phenylanthracen-9-yl)-benzo[b]fluoreno[3,4-d]thiophene derivatives via Suzuki cross coupling reaction. OLED devices using these materials were fabricated in the following sequence; ITO (180 nm) / N,N'-di(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (NPB) (50 nm) / Blue emitting materials (30 nm) / bathophenanthroline (Bphen) (30 nm) / Liq (2 nm) / Al (100nm). A device using 7,7-diphenyl-9-(10-phenylanthracen-9-yl)-7H-benzo[b]fluoreno[3,4-d]thiophene showed the efficient emission, with a luminous efficiency, a power efficiency, and external quantum efficiency of, and the CIE coordinates of 1.79 cd/A, 1.51 lm/W, 3.29 % at 20 mA/cm², and (0.15, 0.09) at 8 V, respectively.

Poster Presentation : **ORGN.P-296**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Phenylanthracene-substituted Indenoquinoline Derivatives for Blue Organic Light Emitting Diodes

Jinho Park, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

In this study, we designed and synthesized blue fluorescent materials based on phenylanthracene-substituted Indenoquinoline. To characterize their electroluminescent properties, multilayered OLEDs were fabricated in the following sequence: indium-tin-oxide (ITO, 150 nm)/4,4',4''-tris[2-naphthyl(phenyl)amino (2-TNATA, 30 nm)/4,4'-bis(N-(1-naphthyl)-N-phenylamino) biphenyl (NPB, 20 nm)/Blue emitting materials (20 nm)/Bathophenanthroline (Bphen, 30 nm)/lithium quinolate (Liq, 2 nm)/Al (100 nm). All devices showed blue emissions with high electroluminescent efficiencies. In particular, a device using 2,7,7,13,13-pentamethyl-9-(10-phenylanthracen-9-yl)-7,13-dihydrobenzo[5,6]-s-indaceno[1,2-g] quinolone exhibited luminous efficiency, power efficiency, and external quantum efficiency of 4.04 cd/A, 1.71 lm/W, 4.51% at 20 mA/cm², respectively, with Commission Internationale d'Éclairage (CIE) coordinates of (0.15, 0.10) at 8.0 V.

Poster Presentation : **ORGN.P-297**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Phenylanthracene-substituted Spiro-indenopyridine Derivatives as Blue Fluorescent Materials for Organic Light Emitting Diodes

Jun Young Moon, Seung Soo Yoon^{1,*}

Department of chemistry, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

In this study, we designed and synthesized blue fluorescent phenylanthracene-substituted Spiro-indenopyridine derivatives with for organic light-emitting diodes (OLEDs) materials. In order to study their electroluminescent properties, the OLEDs devices were fabricated in the following sequence: indium-tin-oxide (ITO, 180 nm)/4,4',4''-tris[2-naphthyl(phenyl)amino (2-TNATA, 30 nm)/4,4'-bis(N-(1-naphthyl)-N-phenylamino) biphenyl (NPB, 20 nm)/Blue emitting materials (20 nm)/Bathophenanthroline (Bphen, 30 nm)/lithium quinolate (Liq, 2 nm)/Al (100 nm). In particular, a device using 7'-(10-phenylanthracen-9-yl)-spiro-[fluoreno[4,3-b]benzofuran-7,5'-indeno[1,2-b]pyridine] in emitting layer showed luminous efficiency, power efficiency, and external quantum efficiency of 3.11 cd/A, 1.63 lm/W, 2.94% at 20 mA/cm², respectively, with Commission Internationale d'Éclairage (CIE) coordinates of (0.15, 0.12) at 8.0 V.

Poster Presentation : **ORGN.P-298**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Efficient Blue Organic Light Emitting Diodes Based on Phenylanthracene-substituted Indenoarenes

Jeongkyu Woo, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

To improve the efficiencies of organic light emitting diodes (OLEDs), many efforts are made to develop the efficient blue fluorescent material. In this study, fluorescent 9-phenylanthracene-substituted indenoarenes were synthesized via Suzuki coupling. To investigate their electroluminescent (EL) properties, multilayered OLEDs with the following sequence; indium-tin-oxide (ITO) (180 nm) / N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) (50 nm) / emitting material (30 nm) / 4,7-diphenyl-1,10-phenanthroline (Bphen) (30 nm) / lithium quinolate (Liq) (2 nm) / Al (100 nm) were fabricated using these materials as emitters. All the fabricated devices showed blue emission. Particularly, a device using 13,13-dimethyl-11-(10-phenylanthracen-9-yl)-13H-indeno[1,2-l]phenanthrene as a emitting material exhibited efficient emission with a luminous efficiency, a power efficiency, an external quantum efficiency, and CIE coordinates of 3.21 cd/A, 1.68 lm/W, 3.21 % at 20 mA/cm², and (0.15, 0.11) at 6V, respectively.

Poster Presentation : **ORGN.P-299**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Study on Synthesis and Optical Properties of Methyl Salicylate Derivatives with Hetero Aromatic Compounds

Miyeon Yoon, Intae Kim*

Department of Chemistry, Kwangwoon University, Korea

We have studied newly synthesized methyl salicylate derivatives with hetero aromatic compounds. Methyl salicylate and its derivatives are naturally found in plants and foods, and used as ingredients of medicinal products, food, mouthwash, and surrogate of chemical warfare agents. Because methyl salicylate has similar properties with other chemical warfare agents like soman and sulfur mustard, methyl salicylate and its derivatives have important role for surrogate of chemical warfare agents. In this work, we have synthesized new methyl salicylate derivatives with three types of hetero aromatic compounds. The structure of the compounds was identified by ^1H NMR, ^{13}C NMR, and FT-IR spectroscopy. We also posted each UV-*vis* absorption, photoluminescence(PL) spectra for the synthesized compounds. Through this work, we can study comparative properties of methyl salicylate and its new derivatives, and it is expected to widen the application of methyl salicylate derivatives.

Poster Presentation : **ORGN.P-300**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Regioselective Fischer indolization in total synthesis of monoterpene indole alkaloids

Tae-Hong Jeon, Dong-Hyun Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Abstract Previously we have reported a conceptually new synthetic approach that provides general access to the aspidosperma alkaloids (+)-aspidospermidine and (-)-tabersonine.¹ Heating in the presence of catalytic amount of an acid effected the [3,3]-sigmatropic rearrangement reaction en route to the indole product without scrambling of the regiochemistry. This method is based on the regioselective indolization of an ene-hydrazide, which was obtained via a base-catalyzed intramolecular aza-Michael reaction, in situ trapping of the resulting enolate, and subsequent C-N coupling with phenyl hydrazide. Although not overly cumbersome, a care was necessary to prevent the enone from undergoing an acid-catalyzed aza-Michael reaction to generate the cyclohexanone product. Now, we have recently discovered that the formation of the cyclohexanone product can be reversed and in fact used for the regioselective generation of enol triflate. Presented herein is our recent progress on the application of our new protocol toward the efficient synthesis of tabersonine and tubifolidine. References 1. Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.* 2017, 19, 6168-6171.

Poster Presentation : **ORGN.P-301**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

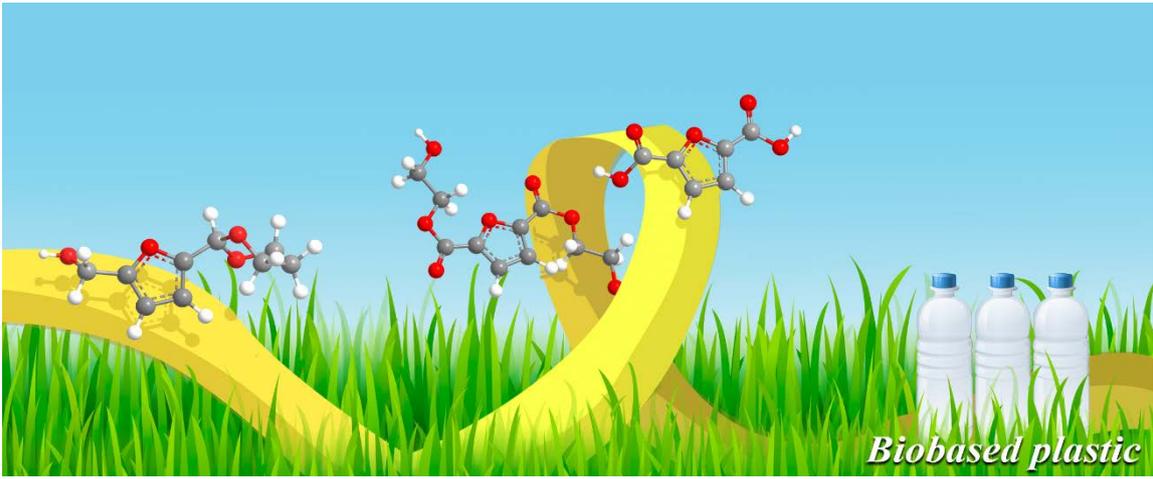
A new route for practical production of furan 2,5-dicarboxylic acid from a cyclic HMF-acetal

Minjune Kim, Yaqiong Su¹, Atsushi Fukuoka, Emiel J. M. Hensen¹, Kiyotaka Nakajima*

Institute for Catalysis, Hokkaido University, Japan

¹*Eindhoven University of Technology, Netherlands*

The utilization of 5-(hydroxymethyl)furfural (HMF) for large-scale production of essential chemicals has been largely limited by the formation of solid humin as a by-product, which prevents the operation of step-wise batch-type processes and continuous flow-type processes. The reaction of HMF with 1,3-propanediol produces an HMF-acetal derivative (PD-HMF) that exhibits excellent thermal stability. The aerobic oxidation of HMF and PD-HMF in water was examined with a CeO₂-supported Au catalyst. When the oxidation was performed using dilute HMF or PD-HMF (1 wt%) solutions in water, FDCA yields for both reactants exceeded 90%. When the concentration of the HMF or PD-HMF reactants was increased to 10 wt%, the results were very different. The FDCA yield from HMF decreased to 28%, whereas it remained as high as 80% with PD-HMF as the reactant. The FDCA yield by PD-HMF oxidation could be further increased to 94% by optimization of the base concentration, however, a similar increase in the base concentration did not further improve the FDCA yield from HMF. It was noted that the higher FDCA yield is largely due to a more complete mass balance, which indicates that by-product formation is significantly suppressed in the presence of two equivalents of base relative to PD-HMF. A further increase of the PD-HMF concentration to 20 wt% only slightly affected the FDCA yield (91%). These results demonstrate that the cyclic HMF-acetal with 1,3-propanediol reported here is a promising intermediate for selective FDCA production from highly concentrated solutions in excess of 10 wt%. The present results represent a significant advance to overcome an inherent limitation of current catalytic process by the oxidation of HMF to an important monomer for biopolymer production.



Poster Presentation : **ORGN.P-302**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

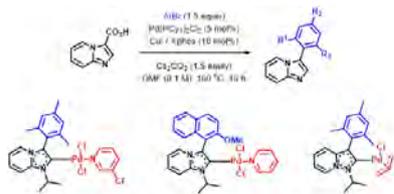
Installation of Sterically Bulky Substituents on Imidazo[1,2-a]pyridine via Decarboxylative Arylation and Development of Abnormal NHC Ligands

Hajoon Kim, Jin Kyoong Park^{1,*}, Haeun Lee¹

Chemistry, Pusan National University, Korea

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

Phosphine ligands have been chosen for a long time in the field of organic chemistry especially in C-C cross coupling reactions. However, N-heterocyclic carbenes (NHCs) are widely being replaced as valid alternatives due to their strong σ -donating capability and higher stability towards air and moisture.^{1,2} Although various modifications of N-substituents on NHC backbone are accessible, very few with the sterically bulky C-substituents have been reported due to their synthetic limitations. As a result of our continuous research on the development of novel abnormal NHC ligands, we found good reaction conditions for C-3 arylation of imidazo[1,2-a]pyridine backbone especially with sterically bulky substituent. Pd/Cu-catalyzed decarboxylative arylation was suitable to install a wide range of sterically bulky substituents. And stable Pd and Rh complexes of imidazo[1,2-a]pyridines were synthesized through the transmetalation of their Ag complex. And the measurement of the CO stretching frequency of dicarbonyl Rh-imidazo [1,2-a]pyridine turned out that our abnormal NHC has lower TEP value (TEP: 2035.7 cm⁻¹) than other known normal NHCs. Many of Pd complexes have been prepared and are being tested in C-C coupling reactions. Furthermore, the complexations with other transition metals, such as, Rh, Ru and Ir are being under investigation.



Poster Presentation : **ORGN.P-303**

Organic Chemistry

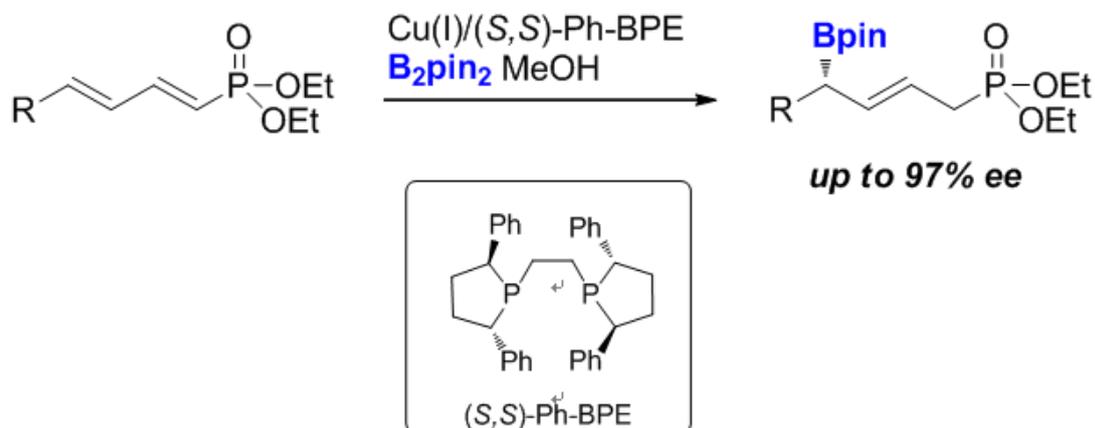
Exhibition Hall 2, THU 11:00~12:30

Enantioselective 1,6-Borylation of 1,3-Dienylphosphonates with Copper-Ph-BPE Catalyst.

Hyesu Lee, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

We have developed copper-catalyzed asymmetric 1,6-borylation of 1,3-dienylphosphonates with B₂pin₂. (S,S)-Ph-BPE was efficient in producing δ -borylated allylphosphonates with high regio- and enantioselectivities up to 97%. Changing the geometry of 1,3-dienylphosphonates from (1E,3E) to (1E,3Z) resulted in formation of the final products with exact opposite absolute configuration and similar enantioselectivities. Further transformation of resulting products such as allylation with aldehydes and cyclization provided a synthetic method for interesting compounds.



Poster Presentation : **ORGN.P-304**

Organic Chemistry

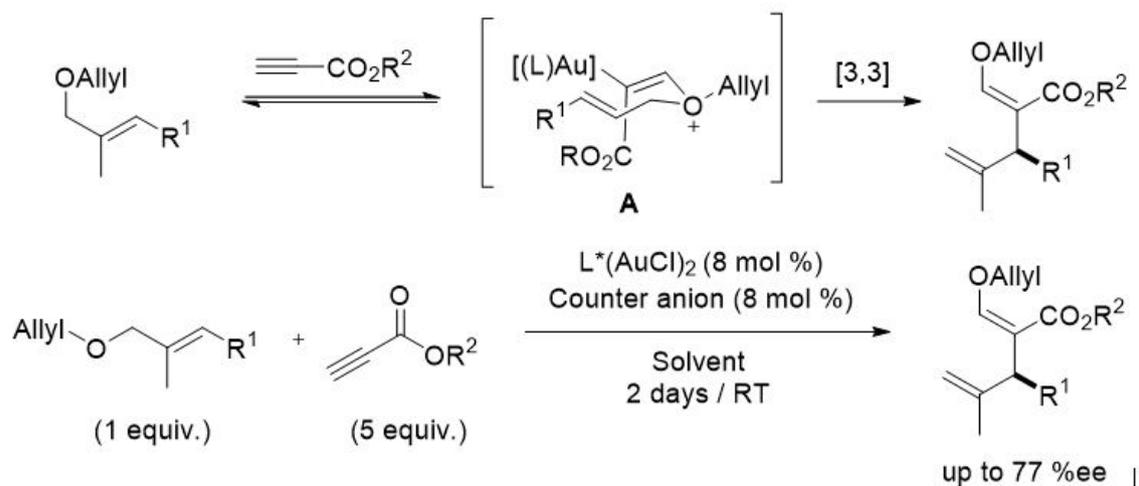
Exhibition Hall 2, THU 11:00~12:30

Intermolecular Enantioselective Carboalkoxylation via Gold(I)-Catalyzed [3,3]-Sigmatropic Rearrangements

Kim Hanbyul, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Claisen rearrangement is a powerful reaction in the construction of carbon–carbon bonds. Gold(I)-catalyzed nucleophilic hydroalkoxylation reactions of alkynes are well-known in modern organic synthesis. In our previous work, we reported in 2013 that the oxonium intermediate formed from allylic ethers underwent [3,3]-sigmatropic rearrangement in the presence of a cationic gold(I) catalyst.¹ Recently, we revisited the enantioselective version of [3,3]-sigmatropic rearrangement transformation with propiolates and allyl ethers. Gold catalyzed asymmetric Claisen rearrangement is challenging because the rearrangement presumably proceeds through a chair transition state where a linearly coordinated alkyne-gold(I) complex lies away from the chiral ligand. Contrary to our expectation, we found that enantio-determining step is the formation of oxonium intermediate **A**, rather than [3,3]-sigmatropic rearrangement. For example, the reactivity and enantioselectivity was highly dependent on the alkoxy group, and among them, O-allyl group turned out to return the best selectivity. With the combination of Josiphos and 1,2,3-trichloropropane, upto 77 %ee was obtained.²References:1. (a) Jun, J.; Yeom, H. –S.; An, J. –H.; Shin, S. *Beilstein J. Org. Chem.* **2013**, *9*, 1724; (b) Park, S. R.; Kim, C.; Kim, D. –G.; Thrimurtulu, N.; Yeom, H. –S.; Jun, J.; Shin, S.; Rhee, Y. H., *Org. Lett.* **2013**, *15*, 1166.2. Kim, H. Jang, J. unpublished work.



Poster Presentation : **ORGN.P-305**

Organic Chemistry

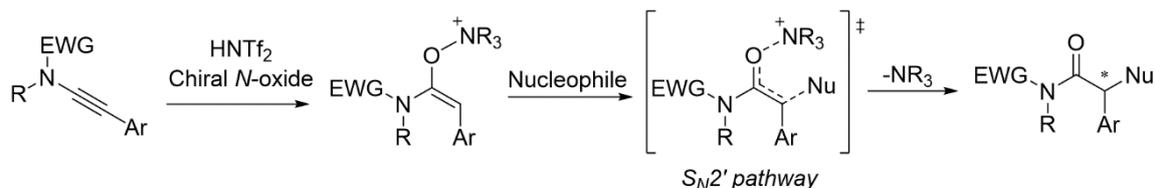
Exhibition Hall 2, THU 11:00~12:30

Brønsted Acid Catalyzed Oxygenative Chirality Transfer via S_N2' -type Coupling of Ynamides

Tae-Woong Um, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Oxygenative coupling of ynamide with external nucleophiles furnishes efficient pathway introducing α -functionalized carbonyl compound. Oxidation of ynamide has been known with pyridine-*N*-oxide under transition metal catalysts, such as Au, Pd catalysis (α -oxo metal carbene pathway),¹ or under Lewis acid (Zn or BARF) or Brønsted Acid (HNTf₂) catalysis (S_N2' pathway).² However, none of these methods allow for an enantioselective access to the products, except in an auxiliary-based approach.³ Herein, we report our preliminary study on the reagent-controlled chirality transfer reaction,⁴ using chiral *N,N'*-dioxide. This process is catalyzed by HNTf₂ (10 %) and affords α -indolyl amides in upto 91 % *ee*. The level of chirality transfer is highly dependent on the mechanism which, in turn, depends on the oxidant (pyr-*N*-oxides or sulfoxides) or substrates (enynamides, ynamides) type. References 1. (a) L. Li, C. Shu, B. Zhou, Y.-F. Yu, X.-Y. Xiao, L.-W. Ye, *Chem. Sci.* **2014**, *5*, 4057. (b) Y. Gao, G. Wu, Q. Zhou, J. Wang, *Angew. Chem. Int. Ed.* **2018**, *57*, 2716. 2. (a) F. Pan, X.-L. Li, X.-M. Chen, C. Shu, P.-P. Ruan, C.-H. Shen, X. Lu, L.-W. Ye, *ACS Catal.* **2016**, *6*, 6055. (b) D.V. Patil, S. W. Kim, Q. H. Nguyen, H. Kim, S. Wang, T. Hoang, S. Shin, *Angew. Chem. Int. Ed.* **2017**, *56*, 3670–3674. 3. (a) A. de la Torre, D. Kaiser N. Maulide, *J. Am. Chem. Soc.* **2017**, *139*, 6578. (b) B. Peng, D. Geerdink, N. Maulide, *J. Am. Chem. Soc.* **2013**, *135*, 14968. 4. Chiral sulfoxide-mediated oxidation has been demonstrated in an intramolecular process: D. Kaldre, B. Maryasin, D. Kaiser, O. Gajsek, L. González, N. Maulide, *Angew. Chem. Int. Ed.* **2017**, *56*, 2212.



Poster Presentation : **ORGN.P-306**

Organic Chemistry

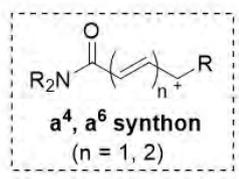
Exhibition Hall 2, THU 11:00~12:30

Generation of Dienolonium Species from Brønsted Acid Catalyzed Oxidation of Enynamides by DMSO: Remote Functionalizations with Carbon and Heteronucleophiles

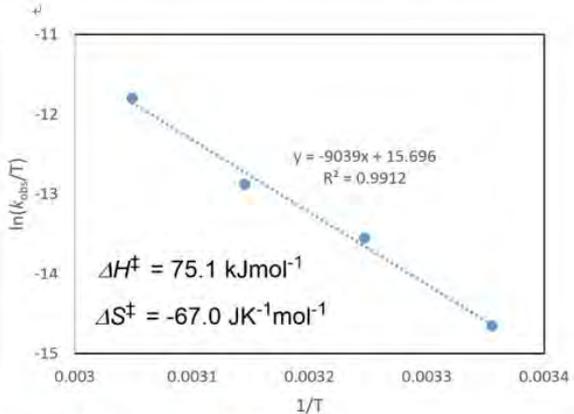
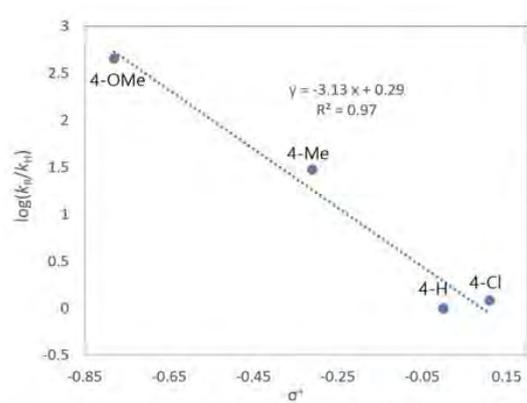
Huong Quynh Nguyen, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Recently we have developed a robust Brønsted acid-catalyzed activation of ynamides enabling oxidative coupling of diverse carbon nucleophiles.¹ As an extension, we envisioned the oxidation of enynamide that would represent an umpolung of silyl dienol ethers in Mukaiyama alkylation. Employing DMSO as the terminal oxidant, oxidative coupling of enynamides efficiently furnished γ -substituted- α,β -unsaturated imides. Furthermore, not only carbon- but heteronucleophiles, such as alcohol, thiol, hydrazides could be employed in this oxidation protocol. In Hammett analysis, the reaction displayed a linear correlation with σ^+ parameters with $\rho = -1.3 \sim -3.1$, indicating the reaction proceeds through a cationic dienolonium intermediate, and the origin of the remote site-selectivity could be ascribed to the charge-development at the terminal carbon. Eyring analysis led us to identify the formation of keteniminium ion as the rate-determining step.²References1. a) D. V. Patil, S. W. Kim, Q. H. Nguyen, H. Kim, S. Wang, T. Huang, S. Shin, *Angew. Chem. Int. Ed.* **2017**, *56*, 3670; b). S.W. Kim, T.W. Um, S. Shin, *Chem. Commun.* **2017**, *53*, 2733.2. Q. H. Nguyen, N. H. Nguyen, H. Kim, Shin, S. manuscript in preparation.



- Regioselectivity: C2, or C4?
- DMSO as a terminal oxidant
- Nu-H: indoles, silyl enol ethers, 1^o, 2^o (thio)alcohols, and hydrazides



Hammett correlation and Eyring analysis



Poster Presentation : **ORGN.P-307**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Progress toward asymmetric total synthesis of bridged indole alkaloids with medium sized ring via regioselective Fischer indolization

Jang yeop Kim, Hyung Joon Kang, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Because of the complex architecture and important biological activities, the Iboga family indole alkaloids have received of particular attention of synthetic organic chemists. While most of these alkaloids have characteristic pentacyclic skeleton bearing indole and isoquinuclidine ring fused by a seven-membered C ring, there exists a small subgroup of natural alkaloids that have a medium sized C ring system embedded in bridged 1-azabicyclo-[6.3.1]dodecane framework. As a part of our ongoing study on regioselective Fischer indolization reaction¹, we have envisaged a new synthetic plan to those 16,21-seco iboga alkaloids. Presented herein is our recent progress toward the asymmetric synthesis of cleavamine.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-308**

Organic Chemistry

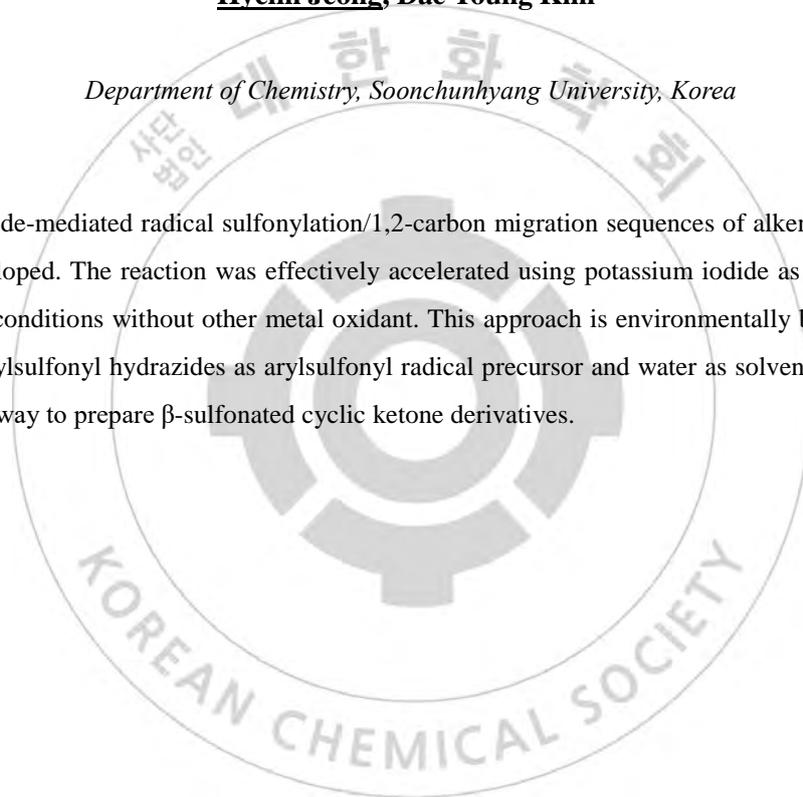
Exhibition Hall 2, THU 11:00~12:30

Synthesis of β -sulfonated cyclic ketones via potassium iodide-mediated radical sulfonylation/semipinacol rearrangement sequences

Hyeim Jeong, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

Potassium iodide-mediated radical sulfonylation/1,2-carbon migration sequences of alkenylcyclobutanols has been developed. The reaction was effectively accelerated using potassium iodide as a catalyst under mild reaction conditions without other metal oxidant. This approach is environmentally benign by use of shelf-stable arylsulfonyl hydrazides as arylsulfonyl radical precursor and water as solvent. This approach offers a facile way to prepare β -sulfonated cyclic ketone derivatives.



Poster Presentation : **ORGN.P-309**

Organic Chemistry

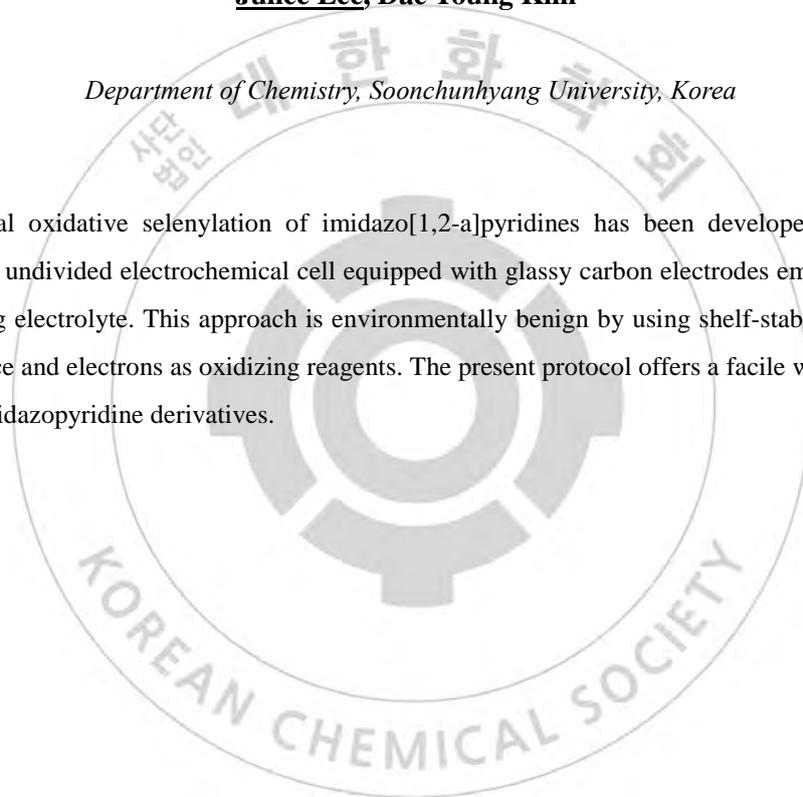
Exhibition Hall 2, THU 11:00~12:30

Synthesis of 3-selenylated imidazopyridins via electrochemical oxidative selenylation of imidazo[1,2-a]pyridines with diselenides

Juhee Lee, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

Electrochemical oxidative selenylation of imidazo[1,2-a]pyridines has been developed. The reaction proceeds in an undivided electrochemical cell equipped with glassy carbon electrodes employing LiClO₄ as a supporting electrolyte. This approach is environmentally benign by using shelf-stable diselenides as selenium source and electrons as oxidizing reagents. The present protocol offers a facile way to prepare 3-selenylated imidazopyridine derivatives.



Poster Presentation : **ORGN.P-310**

Organic Chemistry

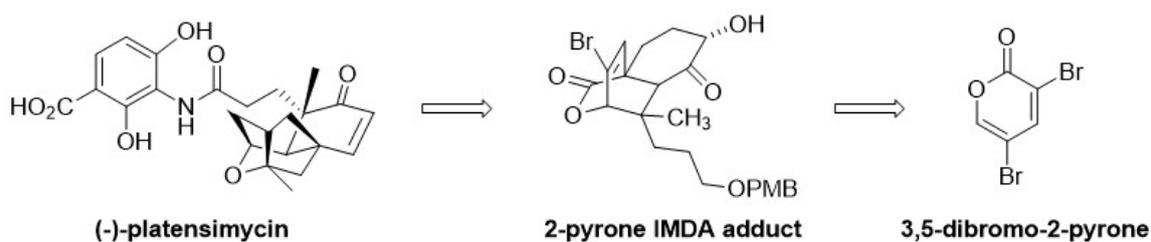
Exhibition Hall 2, THU 11:00~12:30

Progress toward total synthesis of (-)-platensimycin by internal H-bonding mediated intramolecular Diels-Alder reaction

Hyo-mi Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Abstract 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 resulted in successful syntheses of an array of biologically important natural products.¹ Inspired by our recent success on internal hydrogen bonding mediated asymmetric Diels-Alder reaction, we have launched a program inventing a new route that allows an efficient synthesis of (-)-platensimycin. Included in the new route are C3-selective Sonogashira 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-311**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Microscopic observation of kinetic hydrogen isotope separation by the 2nd breathing transition in MIL-53

Minji Jung, Jaewoo Park, Hyunchul Oh^{1,*}

Department of Energy Engineering, Gyeongnam National University of Science and Technology, Korea

¹*Department of Energy Engineering, Gyeongnam National University of Science and Techn, Korea*

Structural flexibility is a unique property of some metal-organic frameworks (MOFs) that clearly distinguishes them from other inorganic porous materials. A MIL-53(Al), one of the most well-known flexible MOF, leads to dynamic changes as closed pore transitions to open pore, also called 'breathing' phenomenon. During the flexible and reversible transition, the pore apertures are continuously adjusted, thus providing the tremendous opportunity to separate mixtures of hydrogen isotope that require precise pore tuning. Recently, we have reported a strategy for effectively separating hydrogen isotopes through the breathing of MIL-53(Al). (JACS, 139(49), 17743-17746, 2017) Typical isotherm of MIL-53 is known to exhibit one-step structural transition from a closed pore to an opened pore structure reversibly by adsorbing different guest molecules. In this study, however, it is newly discovered by our group that the additional D₂ adsorption (30% enhanced uptake) is observed below 25K, leading to the 2nd step breathing transition. Owing to this novel 2nd step breathing transition, D₂ in 1:1 H₂/D₂ mixture is adsorbed solely on MIL-53 at high pressure, leading to the highest separation factor. This phenomenon and isotope separation efficiency are confirmed by advanced cryogenic thermal desorption spectroscopy (acTDS) and also neutron powder diffraction pattern.

Poster Presentation : **ORGN.P-312**

Organic Chemistry

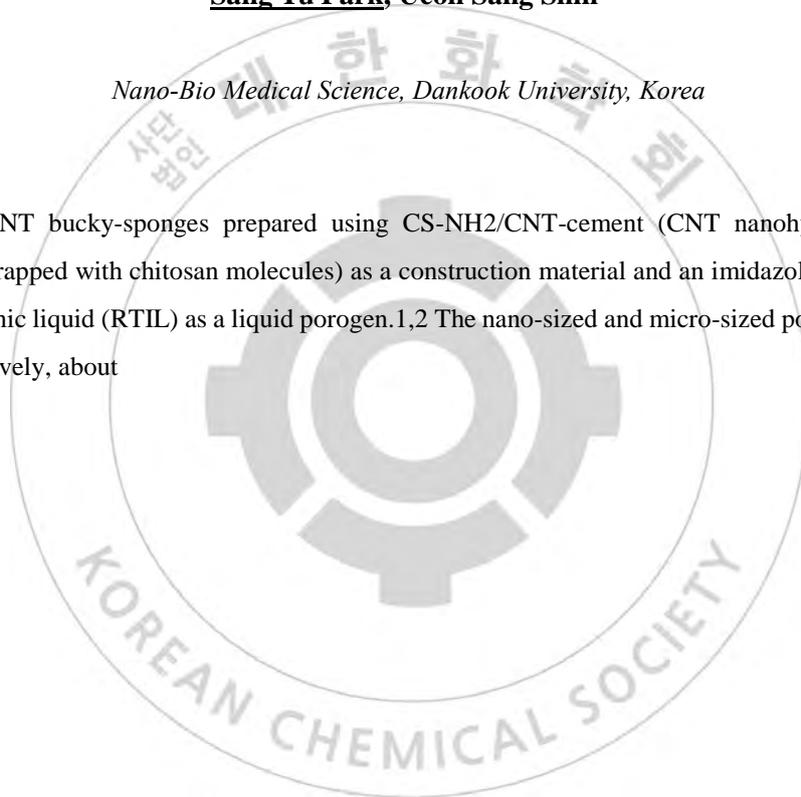
Exhibition Hall 2, THU 11:00~12:30

Highly Porous CNT/Polymer Hybrid Membranes For Heat Signal-Responsive Drug Delivery

Sang Yu Park, Ueon Sang Shin*

Nano-Bio Medical Science, Dankook University, Korea

We present CNT bucky-sponges prepared using CS-NH₂/CNT-cement (CNT nanohybrid molecules individually wrapped with chitosan molecules) as a construction material and an imidazolium based room temperature ionic liquid (RTIL) as a liquid porogen.^{1,2} The nano-sized and micro-sized pores with various width (respectively, about



Poster Presentation : **ORGN.P-313**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

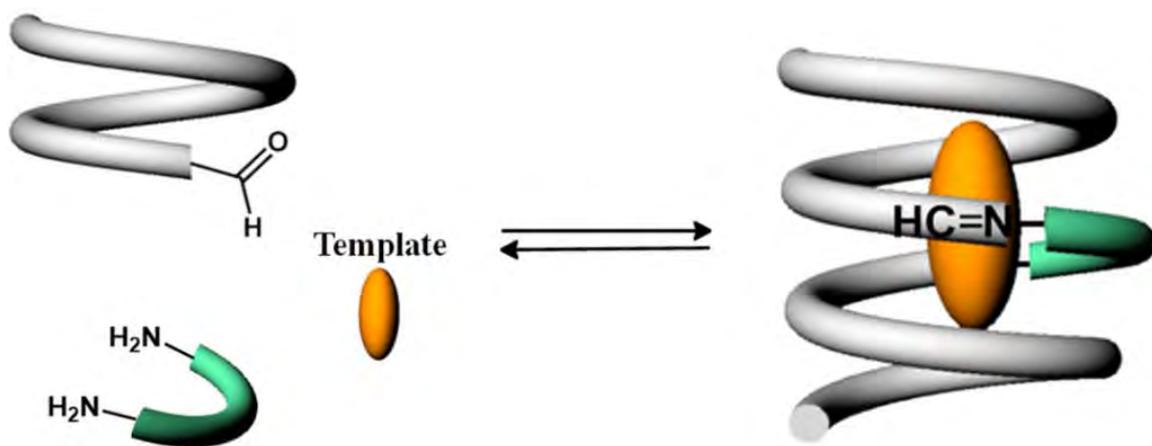
Selective Encapsulation of Tartaric Acid in to a Cavity of Site-Specifically Modified Indolocarbazole-Pyridine Foldamer via Reversible Imine Bonds

Kyungmog Kim, Kyu-Sung Jeong^{1,*}

Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

In recent years, we have demonstrated that indolocarbazole and pyridine (IP) oligomers fold into a helical structure with an internal tubular cavity. The IP foldamers have been subjected to site-specific modification to serve as synthetic receptors for binding specific guests, but the stepwise and covalent modification are tedious and of great challenge. We here present an alternative method for the development of synthetic receptors using the guest-templated synthesis of the IP foldamer via reversible imine bonds. When a short tetramer with an aldehyde group at one end is mixed with 1,3-diaminobenzene in the presence of various carboxylic acids, a mixture of the two reactants, monoimine and diimine monoimine exist in solution. Among more than 20 chiral or achiral carboxylic acids we examined, D- or L- tartaric acid results in the complete formation of only one imine-linked foldamer without any side-product. The resulting imine foldamer adopts a helical conformation with an internal cavity in which D- or L- tartaric acid is tightly encapsulated. All details including by NMR spectroscopic and circular dichroism (CD) data will be further described in the presentation



Poster Presentation : **ORGN.P-314**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Scalable Synthetic Route for Mono-functionalized CB[7] derivatives

Suman Kumar Ghosh, Moon Young Hur, Young Ho Ko, Kyeng Min Park*, Kimoon Kim^{1,*}

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

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

Cucurbit[7]uril (CB[7]) is a pumpkin shaped macrocyclic host molecule, well-known for exceptionally high binding affinity to its guest such as adamantyl- and ferrocenyl- ammonium ($K_a > 10^{13} \text{ M}^{-1}$). Recently, mono-functionalization of CB[7] conjugated to fluorescent dyes and polymer beads provided new applications of CB technology for bioimaging and proteomics. However, low yield of mono-functionalized CB[7] has limited their practical applications. Here, we report a scalable synthetic route to produce mono-functionalized CB[7] in high yield using acid-mediated one pot reaction. Monohydroxy-CB[7] was efficiently transformed to monocarboxylated-CB[7] in a quantitative manner. In addition, this synthetic methodology was useful for other functionalities on CB[7] such as azide and acrylate for click and Michael reaction, respectively. This synthetic route may expand the scope of CB[7] to practical applications for materials and biomedicines. References: 1. Kim, K.; Murray, J.; Selvapalam, N.; Ko, Y. H.; Hwang, I., Cucurbiturils. World Scientific (Europe): 2018. 2. Kim, K.; Selvapalam, N.; Ko, Y. H.; Park, K. M.; Kim, D.; Kim, J. Chem. Soc. Rev. 2007, 36, 267-279. 3. Shetty, D.; Khedkar, J. K.; Park, K. M.; Kim, K. Chem. Soc. Rev. 2015, 44, 8747-8761. 4. Li, M.; Lee, A.; Kim, K. L.; Murray, J.; Shrinidhi, A.; Sung, G.; Park, K. M.; Kim, K. Angew. Chem. Int. Ed. 2018, 57, 2120-2125. 5. Kim, K. L.; Sung, G.; Sim, J.; Murray, J.; Li, M.; Lee, A.; Shrinidhi, A.; Park, K. M.; Kim, K., Nat. Commun. 2018, 9, 1712.

Poster Presentation : **ORGN.P-315**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

The Effect of Remote Chlorine Substituent on the Kinetic Resolution of *cis*-Vinyl Epoxide via Chiral Lewis Base-Catalyzed Ring Opening

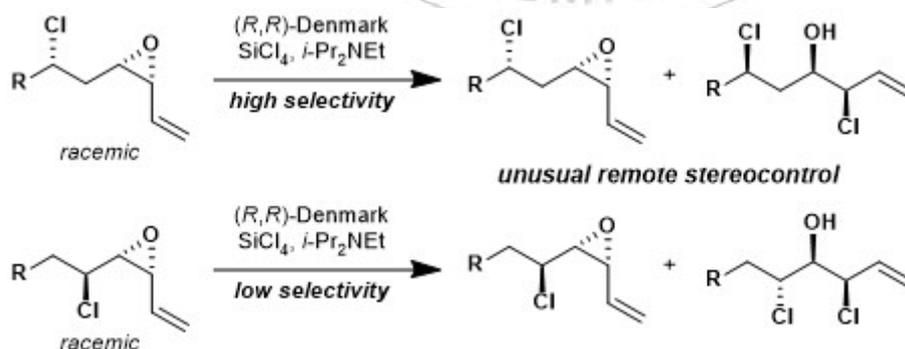
Jungi Jung, Won-jin Chung*

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

Substrate-controlled, relative stereoselection typically utilizes an adjacent stereocenter in close proximity. On the other hand, the influence of a remote stereocenter is generally less significant. When our group set out to study the effect of chlorine substituents on the kinetic resolution of *cis*-vinyl epoxide,¹ it was anticipated that the stereoselectivity would be controlled primarily by the α -chlorine substituent. However, counterintuitively, the dominant role of the β -chlorine substituent was observed instead. Here, we report the result of our investigation and a possible explanation for the unusual remote stereocontrol.

References

- (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.



Poster Presentation : **ORGN.P-316**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Denitrogenative Ring Contraction of 1,4-Dimethoxyphthalazines

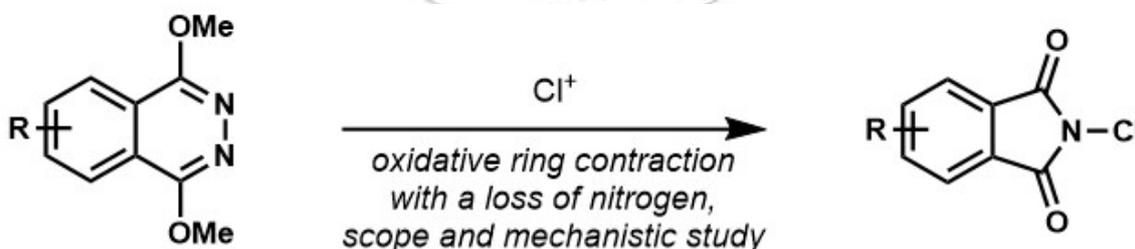
Jeong Kyun Im, Ilju Jeong, Won-jin Chung*

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

Our group has been investigating *N*-halogenation of heterocyclic compounds. While attempting *N*-chlorination of 1,4-dimethoxyphthalazine, unexpected ring contraction took place via a loss of one nitrogen atom to give *N*-chlorophthalimide. Although a few examples of related ring contraction of phthalazine-1,4-dione were reported several decades ago,^{1,2} this type of denitrogenative ring contraction has never been systematically studied. Moreover, the detailed reaction mechanism is still unknown. We are currently examining the substrate scope with a wide range of electronically diverse 1,4-dimethoxyphthalazine derivatives. In addition, a plausible reaction mechanism was proposed on the basis of the observed reaction intermediate.

References

1. Parrick, J.; Ragunathan, R. *J. Chem. Soc., Perkin Trans. 1*, **1993**, 211-216.
2. Omote, Y.; Yamamoto, H.; Sugiyama, N. *J. Chem. Soc. D*, **1970**, 914.



Poster Presentation : **ORGN.P-317**
Organic Chemistry
Exhibition Hall 2, THU 11:00~12:30

Stereoselective Cycloadditions for a Series of N-Heterocycles: Beyond Corey-Chaykovsky Reactions

Jiyoun Lee, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Korea

Cyclopropane-containing systems, especially cyclopropane fused N-heterocycles, are common structural motives in many natural products, pharmacophore, and functional molecules. Besides, a three-membered ring can undergo a variety of transformations, such as ring openings, ring expansions, or cycloadditions resulting in furnishing complex structures. However, the synthetic approach of cyclopropanes has mostly relied on the carbene transformation using an expensive rhodium catalyst. Notably, stereoselective cyclopropanation under the catalyst-free conditions remains an unexplored field. Recently, we discovered that N-aromatic zwitterions could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5 + n] cycloadditions with electrophilic partners. Based on our previous results, in this symposium, we will discuss diastereo- and enantioselective cyclopropanations through catalyst-free reactions between quinolinium zwitterions and various 1C coupling partners (sulfonium and sulfoxonium ylides). Interestingly, depending on the nature of coupling ylides, a variety of cycloadducts can be prepared stereoselectively.

Poster Presentation : **ORGN.P-318**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Two-photon ratiometric Probe for Quantitative analysis of hNQO1 enzyme Activity in Colorectal cancer.

Myoung Ki Cho, Hwan Myung Kim^{1,*}

Energy systems research, Ajou University, Korea

¹*Energy Systems Research, Ajou University, Korea*

Human NAD(P)H:quinone oxidoreductase 1(hNQO1, E.C.1.6.99.2.) as a flavoenzyme catalyzes two- or four-electron reduction of endogenous and exogenous quinones to their hydroquinone forms.¹ Reductions catalyzed by hNQO1 play an important role in cell protecting, detoxification and antioxidant cycle.¹ hNQO1 is over-expressed in tumor cells compared with normal cells of the same origin. Especially, human colonic carcinomas show a markedly increase activity of hNQO1.² In this work, we developed ratiometric two-photon fluorescence probe for quantitative detection of hNQO1 activity in human cancer and normal tissues. The ratiometric system that change emission wavelength activated with enzyme produces precise quantitative analysis of hNQO1 activity in different samples through dual channel monitoring unlike the turn-on system.³ Two-photon microscopy (TPM) employs two near-infrared photons as the excitation source, offers a number of advantages including greater penetration depth (> 500 μm), localization of excitation with minimum background signal, and longer observation times.⁴ This ratiometric two-photon fluorescent probe shows perceptible blue-to-yellow emission wavelength change activated with hNQO1, high stability and selectivity. This probe can monitor the activity of hNQO1 quantitatively in living cells and human colon tissue. References 1. Nebert, D.W.; Roe, A.L.; Vandale, S.E.; Bingham, E.; Oakley, G.G. *Genet. Med.* 2002, 4, 62-70. 2. Schor, N.A.; Cornelisse, C.J. *Cancer Res.* 1983, 43, 4850-4855. 3. Lee, H.W.; Heo, C.H.; Sen, D.; Byun, H.O.; Kwak, I.H.; Yoon, G.; Kim, H.M. *S. A. Anal Chem.* 2014, 86, 10001-10005. 4. Kim, H.M.; Cho, B. R. *Chem. Rev.* 2015, 115, 5014-5055.

Poster Presentation : **ORGN.P-319**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

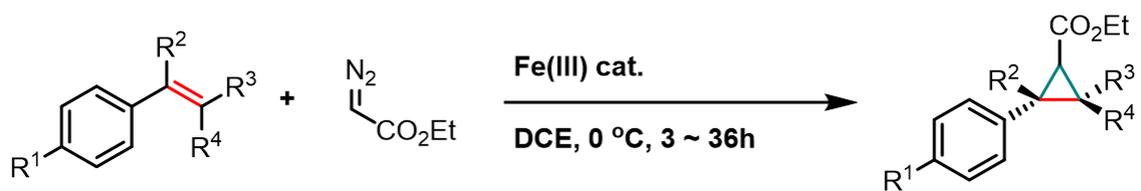
Radical Cation Cyclopropanation Reaction using Iron(III)-polypyridyl Complex

Yong hyun Cho, Kwang-Hyun Ahn¹, Eun Joo Kang^{1,*}

Chemistry, Kyung Hee University, Korea

¹*Department of Applied Chemistry, Kyung Hee University, Korea*

Various cyclopropanation of diazo reagent with electron-rich alkene have been studied for its reaction through metal carbenoid of Ru, Rh and Fe. However, the redox reaction through a single electron transfer has been rarely reported. The Ferreira group reported the chromium photocatalyzed cyclopropanation reaction of alkene, which was transformed to the radical cation intermediate by single electron oxidation process. Iron(III)-polypyridyl complexes also have the adequate potential ($E_{1/2} = +0.82\sim 1.10$ V) to oxidize electron-rich alkenes such as anethole and stilbene ($E_{1/2} = +1.10\sim 1.61$ V) to form alkene radical cation intermediates. Under optimal condition of Fe(III)-polylyridyl complex, various cyclopropanes were synthesized from anetholes or stilbenes with different diazo esters. The mechanism of the radical cation cyclopropanation reaction was investigated by DFT calculation and several mechanistic experiments. Fe(III) catalyst oxidize anethole or stilbene to corresponding radical cation intermediate by single electron transfer, and the resulting radical cation reacts with a nucleophilic diazo ester. Simultaneous loss of N_2 affords a long-bonded cyclopropane radical cation. This reaction can be green and effective method using inexpensive iron to afford a radical cation cyclopropanation reaction. **Acknowledgement** This study was supported by the Ministry of Education, Science and Technology, National Research Foundation (Grant No. 2018R1A2B6008824). **References** (1) (a) Sarabia, F. J.; Ferreira, E. M. *OrganicLetter* **2017**, *19*, 2865–2868; (b) Shin, J. H.; Seong, E. Y.; Mun, H. J.; Jang, Y. J; Kang, E. J. *OrganicLetter* **2018**, *20*, 5872-5876. (2) Yueh, W.; Bauld, N. L. *J.Am.Chem.Soc* **1995**, *117*, 5671-5676.



R¹ = OAlkyl, H
R², R³ = Alkyl
R⁴ = Alkyl, Ar



Poster Presentation : **ORGN.P-320**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Cyclic Carbonate from CO₂ and Epoxide Catalyzed by Heteroleptic Fe(II)-iminopyridine Complexes

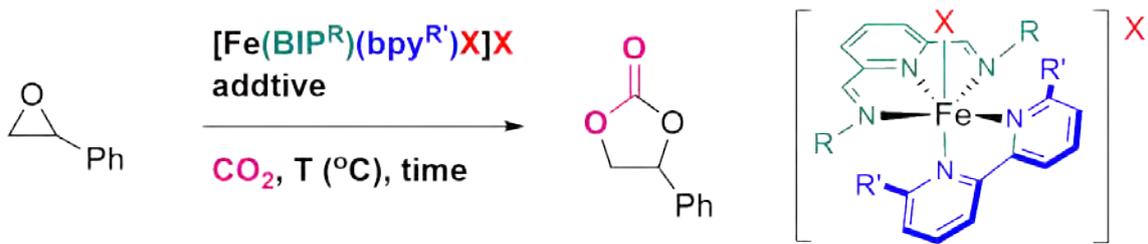
Namhee Kim, Jae Hyung Kim, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Iron complexes, one of the abundant first-row transition metal catalysts, have been used to couple epoxide and CO₂ to afford cyclic carbonate. In the synthesis of cyclic carbonates from epoxides, the epoxide ring opening can be facilitated by a Lewis-acidic metal catalyst or a Brønsted-acidic organocatalyst having an OH or NH group.¹ While studies on epoxide activations have been active, research on CO₂ activations has lagged a bit. CO₂ activation is possible by Lewis bases such as amine, alcohol, and *N*-hetero aromatic compound.² Due to the electrophilic nature of the carbon atom of CO₂, electron-rich nucleophiles participate in forming the CO₂-adduct, and the solubility of CO₂ is increased in the zwitter-ionic form of CO₂-adduct. While multifunctional Fe(II) complexes containing Lewis acidic metal centers, hydrogen bonding donors and nucleophilic halides were developed in previous studies,^{1b} in this work, new multifunctional Fe(II) complexes were designed to synthesize cyclic carbonate under mild conditions by introducing Lewis base. The heteroleptic Fe(II) complexes are capable of CO₂ activation by Lewis base-derived ligand and epoxide activation as hydrogen bonding donor are developed. As a result, we could synthesize styrene oxide to cyclic carbonate at low pressure of CO₂ and low reaction temperature under solvent-free condition, and it was possible to make more efficient reaction using additive.

Acknowledgement This study was supported by the Ministry of Education, Science and Technology, National Research Foundation (Grant No. 2017M1A2A2043147 “Next Generation Carbon Upcycling Project”).

References (1) (a) Langa, X.-D.; Yua, Y.-C.; Hea, L.-N. *J. Mol. Catal. A* **2016**, *420*, 208–215; (b) Seong, E. Y.; Kim, J. H.; Kim, N. H.; Ahn, K.-H.; Kang, E. J. *ChemSusChem* **2019**, *12*, 409-415. (2) Al-Qaisi, F. M.; Nieger, M.; Kemell, M. L.; Repo, T. J. *ChemistrySelect* **2016**, *3*, 545-549.



Poster Presentation : **ORGN.P-321**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Mechanochemical polymerization of trimethylene carbonate

Sora Park, Jeung Gon Kim*

Department of Chemistry, Chonbuk National University, Korea

Mechanochemical polymerization of trimethylene carbonate can be realized by using ball milling. In addition to general advantages of mechanochemistry, such as high conversion and solvent free synthetic approaches, our group demonstrate herein the rate acceleration under solid-state polymerization. Among popular organocatalysts, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) and 1,5,7-diazabicyclo[4.4.0]dec-5-ene (TBD) exhibited rate enhancement comparing to those of solution polymerizations. To understand the origin of high efficiency, investigation of the temperature was conducted and revealed that the heat from ball collisions and exothermic energy are not significantly influential on the polymer synthesis rate. Other studies such as liquid-assisted grinding and high-molecular weight polymerization will be presented.

Poster Presentation : **ORGN.P-322**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Use of Phosphite Esters for Exploring S-Nitrosothiol Chemistry

Clovis Shyaka, Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea

The reactions between S-nitrosothiols (SNOs) and phosphite esters, including $P(OPh)_3$, $P(OBn)_3$ and $P(OEt)_3$, were studied. The reaction resulted in two different conjugated adducts, phosphorothioates and thiophosphoramidates, depending on the primary and tertiary structures of S-Nitrosothiols substrates. phosphorothioates were obtained as the main products from primary SNO substrates, while thiophosphoramidates were obtained from tertiary SNOs under mild conditions. Theoretical studies revealed that the reaction between SNOs and phosphite esters could proceed via two reaction pathways and yields the two different conjugated products depending on the structure of SNO compounds. Herein we report an experimental and theoretical investigation on the reaction between phosphites and SNO substrates.

Poster Presentation : **ORGN.P-323**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of A Novel Synthetic Method for Construction of Unsymmetrical Dimeric Indole Compounds

Hyung Joo Kim, Jiye Jeon¹, Cheol-Hong Cheon^{1,*}

Chemistry, Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

The dimeric indole compounds are class of the important structural motifs founded in indole natural products. Among the various dimeric species of indole, the bisindole structure in which two indoles are directly connected by single bond is the privileged scaffold. They exhibit widespread biological activities such as inhibition of protein kinase, cytotoxicity against tumor cell and cytotoxicity against human breast cancer. Because of these useful properties, they have attracted a lot of attention from the synthetic and medicinal communities. To date, several synthetic protocols of these useful structures have been reported in literatures. However, these reported methods have been applicable to a very limited scope of dimeric species. Particularly there have been few methods to access unsymmetric dimeric indole structures. In these reasons, the development of new efficient synthetic protocol is still in need. Very recently, our group developed novel method to construct dimeric compound of indole via the cyanide catalyzed imino-Stetter reaction from 2-aminocinnamic acid and indole-2-carboxaldehyde.¹ When aldimines derived from 2-aminocinnamic acid derivatives and protected indole-2-carboxaldehydes were treated with catalytic amount of cyanide, the desired dimeric compounds were obtained. We further attempted to extend this protocol to the synthesis of dimeric indole compounds bearing different substituents at each indole moiety. The 2-aminocinnamic acid derivatives and indole-2-carboxaldehyde derivatives bearing different substituents gave the unsymmetric dimeric indole compounds. Herein we describe a novel synthetic method to construct unsymmetric dimeric indole compounds. Reference 1. Lee, S.; Kim, K.-H.; Cheon, C.-H.; Org. Lett. 2017, 19, 2785.

Poster Presentation : **ORGN.P-324**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Total synthesis of fimsbactins and investigation of the stereoselectivity of the fimsbactin uptake machinery in *Acinetobacter baylyi* ADP1

Hak Joong Kim*, Soojeung Kim

Department of Chemistry, Korea University, Korea

Siderophores are small molecule iron-chelators secreted by microorganisms in response to iron limitation. When pathogens infect a human, they utilize siderophores to intercept the iron in the infected host system for their proliferation. Therefore, the siderophore is considered as a key virulence factor, suggesting that the mechanisms associated with the siderophore metabolism can be viable antibiotic targets. The issue caused by the infection by *Acinetobacter baumannii*, a Gram-negative pathogen, is particularly problematic due to its rapid development of antibiotic resistance. The low permeability of the outer membrane has been considered as the major contributor to its drug resistance. In this regard, recently many researchers are paying attention to the use of a siderophore as an intracellular antibiotic delivery vehicle as an effective way to overcome the drug resistance associated with the outer membrane barrier. We have been interested in fimsbactins, the siderophore class produced and utilized by *A. baumannii* in addition to its non-pathogenic relative, *Acinetobacter baylyi* ADP1, to exploit its potential as an antibiotic delivery vehicle. Specifically, in this study, the total synthesis of fimsbactin A and B were established. In addition, generation of stereoisomers of those fimsbactin molecules as well as the evaluation of their iron delivery properties were conducted to probe the stereoselectivity of the fimsbactin uptake machinery in *A. baylyi* ADP1. These results will provide significant resources in rational design of fimsbactin-based siderophore-antibiotic conjugates capable of effectively treating drug-resistant *A. baumannii*.

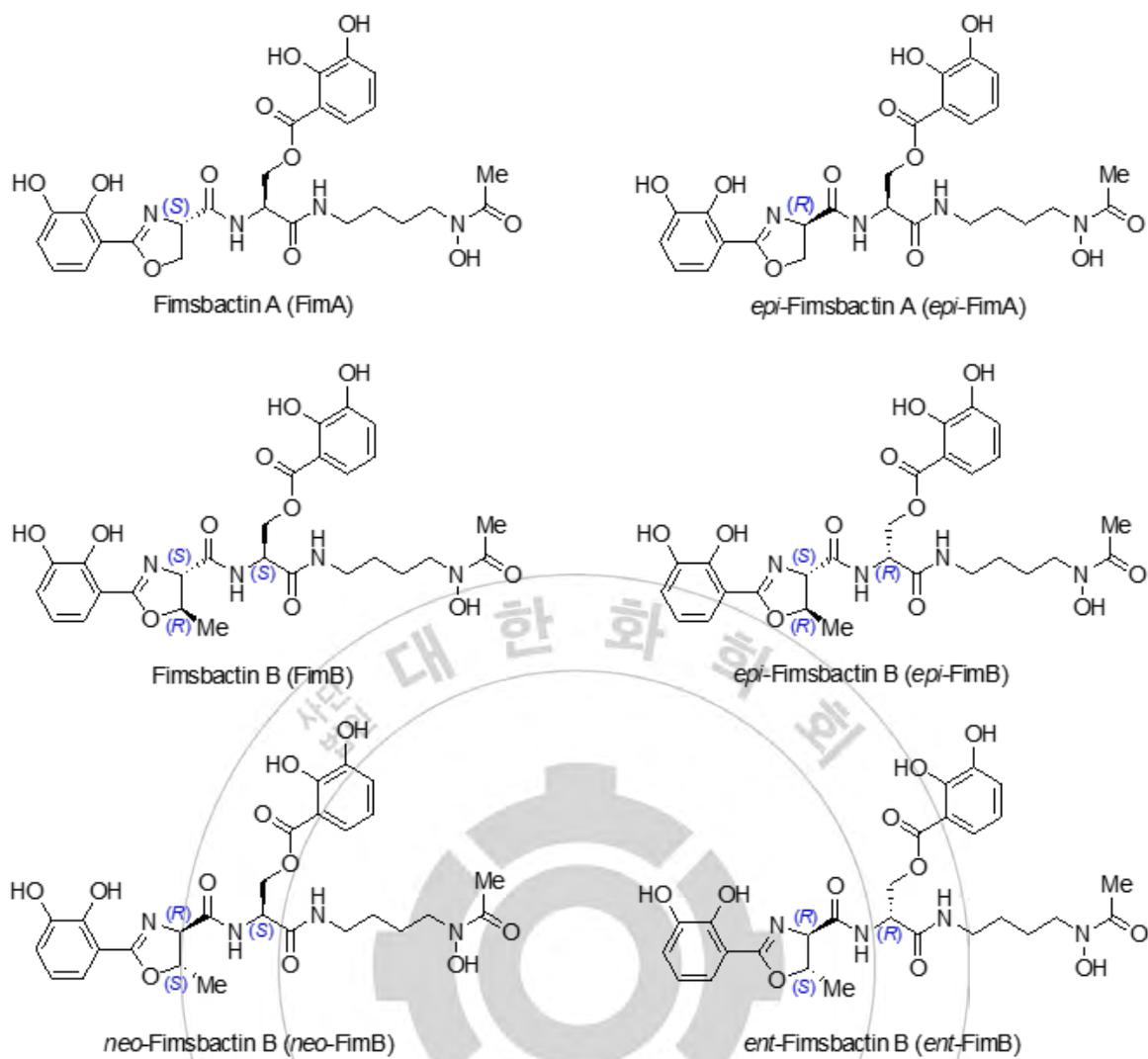


Figure. The structures of fimsbactin A, B, and their stereoisomers

Poster Presentation : **ORGN.P-325**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Amidine-derived Small Two Photon Fluorescent Probes to observe the movement in living cells

Ji Soo Kang, Hwan Myung Kim*

Department of Energy Systems Research, Ajou University, Korea

Vesicle transport plays an important role in the unique proteins and lipid organization of the cell organelles. After protein and lipid synthesis in the endoplasmic reticulum (ER), they are accumulated in the Golgi, and transported to their final destinations through budding and fusion mechanisms¹. The malfunction of vesicle transport leads to a variety of human disorders, such as atherosclerosis and Alzheimer's disease as well as many related genetic diseases^{2,3}. However, the underlying mechanism of the diseases is almost unrecognizable. To provide a genuine monitoring method of vesicular transport, we developed amidine-derived small molecule two-photon fluorescent probes. These probes showed a strong two photon excited fluorescence, good water solubility, pH independency, low cytotoxicity and high cell loading ability. Through these probes, two-photon microscopic imaging experiments show that these probes have various cellular localizing properties and these probes can be an effective tool for studying biology related to human trafficking in real time. References 1. Bannykh, S. I.; Balch, W. E. J. *Cell Biol.* **1997**, *138*, 12. Spady D. K. *Circulation.* **1999**, *100*, 5763. Abad-Rodriguez, J.; Ledesma, M. D.; Craessaerts, K.; Perga, S.; Medina, M.; Delacourte, A.; Dingwall, C.; De Strooper, B.; Dotti, C. G.; *J. Cell Biol.* **2004**, *167*, 953

Poster Presentation : **ORGN.P-326**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A new hydrazine recognition system based on fluorescent sensor array

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³*Division of Chemistry, Seoul National University, Korea*

Hydrazine is an ambivalent chemical, consisted with single-bonded two nucleophilic nitrogen atoms. It is best known as fuel propellant for rocket and spacecraft, and has been also widely used in diverse research areas, including pharmaceutical chemistry, agricultural chemistry, or coordination chemistry. At the same time, however, hydrazine has been considered as a toxic and carcinogenic chemical by U.S. environmental protection agency (EPA), causing damages to liver, kidneys, and central nervous system. Several analytical techniques can be applied for the detection of a hydrazine molecule, such as spectrophotometric, titrimetric, voltammetric, or chromatographic. Among them, fluorescence techniques have multiple advantages over other methods, for example, sensitivity, immediacy, and easy-accessibility. Herein we developed chemical array system for hydrazine recognition with fluorescent array pattern analysis. To generate the array system we developed 4 different fluorogenic probes, SF-Azo 01–04, via introducing azo moiety on versatile fluorescent molecular framework, 9-aryldihydropyrrolo[3,4-b]indolizin-3-one (Seoul-Fluor). We confirmed azo functional group successfully quench the emission of Seoul-Fluor system. Reaction of SF-Azo probes with hydrazine result fluorescence turn on up to 878 fold increase. Simple spotting of the compounds on cellulose paper allowed generating 2x2 fluorescent sensor array, and we could successfully detect and discriminate concentration differences of hydrazine samples with the fluorescent array. This proof of concept study demonstrated the usefulness of under-evaluated azo functional group as a molecular reporter for the hydrazine detection and, more importantly, fluorescent sensor array system is useful for sensing the molecule of interest.

Poster Presentation : **ORGN.P-327**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of 4-hydroxy-2-naphthoic acid, a pharmacologically important drug intermediate

Kyungmin Kim, Hyunjin Lee¹, Hakwon Kim^{1,*}

Department of Chemical Advanced Materials, Kyung Hee University, Korea

¹Department of Applied Chemistry, Kyung Hee University, Korea

6-Deoxymollugin, 4-isoamyl-2-naphthamide derivatives and 1,4-naphthoquinone derivatives are compounds that exhibit various physiological activities. 4-Hydroxy-2-naphthoic acid is a core structure of these biologically important compounds and used as a key intermediate in the synthesis of these final target compounds. The synthesis of 4-hydroxy-2-naphthoic acid is well known, which are 1) Wittig olefination of benzaldehyde and intramolecular cyclization 2) Horner-Wardworth-Emmons reaction of benzaldehyde and intramolecular cyclization 3) Stobbe condensation of benzaldehyde and intramolecular cyclization. However, these synthetic methods are often not applied well to a variety of 4-hydroxy-2-naphthoic acid derivatives such as A-ring substituted derivatives. In this study, three synthetic methods of 4-hydroxy-2-naphthoic acid were studied and their usefulness was compared. And we have studied to find the most suitable synthesis method according to functional group substituted on A ring of 4-hydroxy-2-naphthoic acid.

Poster Presentation : **ORGN.P-328**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Two-photon ratiometric probe for Analyzing Ca^{2+} in live cells and its application in spinal cord injury model

DongJoon Lee, Hwan Myung Kim*

Department of Energy Systems Research, Ajou University, Korea

Intracellular Ca^{2+} ($[\text{Ca}^{2+}]_i$) play a role in controlling various cellular functions.¹ Abnormal $[\text{Ca}^{2+}]_i$ can implicate human disorders such as neurodegeneration, heart disease, and several disease.² Most small molecule probes for Ca^{2+} also limit their applications in live cell imaging due to the turn-on response process, rapid photobleaching, and short wavelength excitation light, which can cause photodamage, and have limited tissue imaging depth. A appropriate approach is the use of an emission ratiometric probe with two-photon microscopy (TPM), which employs two near-infrared photons as the excitation source.³ The TPM has become one of the most influential technique for imaging studies in living systems, owing to its advantages including great tissue penetration depth, localization of excitation, low photo-damage, and longer observation times.⁴ We developed a two-photon ratiometric probe for $[\text{Ca}^{2+}]_i$ in live sample. This probe derived from dual dyes with different Stokes shifts and probe had dual channel, Ca^{2+} sensing window and internal reference window, without FRET interference. This ratiometric probe can analyze quantitative $[\text{Ca}^{2+}]_i$ in live cells and tissues including rat spinal cord tissue. References 1 Emerit, J.; Edeas, M.; Bricaire, F. *Biomed. Pharmacother.* 2004, 58, 39-46. 2 Berchtold, M.W.; Brinkmeier, H.; Münsterner, M. *Physiol. Rev.* 2000, 80, 1215-1265. 3 Helmchen, F.; Denk, W. *Nat. Methods* 2005, 2, 932-940. 4 Kim, H.M.; Cho, B. R. *Chem. Rev.* 2015, 115, 5014-5055.

Poster Presentation : **ORGN.P-329**

Organic Chemistry

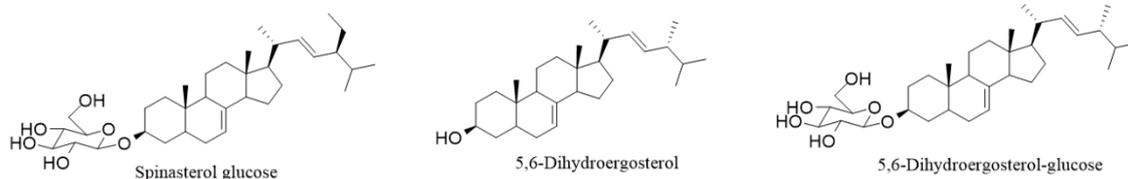
Exhibition Hall 2, THU 11:00~12:30

Synthesis of 3-epi-5,6-Dihydroergosterol and Its Glycosides and Comparison of Anti-inflammatory Activity

Hyunji Kang, Yeseul Park, Hyejin Moon, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Natural spinasterol-glucose (3-O- β -D-glucopyanosylspinasterol), isolated from *Stewartia koreana* leaves, has been identified as a compound to exhibit a potent anti-inflammatory activity. In our previous studies, new steroids structurally similar to spinasterol, such as 5,6-dihydroergosterol (DHE) and ergosterol (Ergn) were developed. The anti-inflammatory activity of DHE, DHE-glycosidies, Ergn and Ergn-glycosides has been already demonstrated, also. This study describes a recent synthesis of 3-epi-DHE and its glycosides and a comparison of anti-inflammatory effects with DHE and DHE-glycosides.



Poster Presentation : **ORGN.P-330**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Two-Photon Fluorescent Probe for Ratiometric Detection of Hydrogen polysulfides and Its Application in Parkinson's Disease

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energy system department, Ajou University, Korea

¹*Department of Energy Systems Research, Ajou University, Korea*

Hydrogen polysulfides (H_2S_n , $n>1$) are Hydrogen sulfide (H_2S) derived signaling molecules that are produced primary during the cross talk between H_2S and reactive oxygen species (ROS)/ reactive nitrogen species (RNS).^{1,2} H_2S_n is mostly generated in the mitochondria, and abnormal mitochondrial function and oxidative stress are directly related to many disorders including Parkinson's disease (PD).³ Therefore, a marker that can directly observe H_2S_n is required to determine its association with the abnormal mitochondrial function observed in many diseases. In this study, we developed a ratiometric TP probe for quantitative measuring H_2S_n in mitochondria and its application to a Parkinson's disease (PD) model to quantify the H_2S_n levels. Using this sensitive selective probe, we observed mitochondrial H_2S_n is generated more in PD neuron than in normal neuron. References 1. Y. Kimura, Y. Mikami, K. Osumi, M. Tsugane, J. I. Oka and H. Kimura, *FASEB J.*, **2013**, 27, 2451-2. T. V. Mishanina, M. Libiad, R. Banerjee. *Nat. Chem. Biol.* **2015**, 11, 4573. H. Kimura. *Molecules*, **2014**, 19, 16146

Poster Presentation : **ORGN.P-331**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A New Infrared Probe Targeting Mitochondria via Regulation of Molecular Hydrophobicity

Eunha Kim^{*}, Jun-Sik Min¹

Department of Molecular Science and Technology, Ajou University, Korea

¹Molecular science and technology, Ajou University, Korea

The morphology of the mitochondria is affected by cell function and disease state. Recent studies indicated that the morphology of the mitochondria can be utilized as a biological marker for the diagnosis of cancer phenotypes and to monitor drug response. So the demand for fluorescent mitochondrial bioprobes has been increasing. For the efficient transfer of probe molecules through lipid bilayers and their accumulation in the mitochondrial matrix, most fluorescent bioprobes targeting mitochondria are based on compound conjugation with lipophilic cations (typically triphenyl phosphonium ion). Herein, using 10 commercial amines as additives to modify the hydrophobicity of Si-R fluorescent cores, we have developed near-infrared (NIR) fluorescent probes for mitochondrial staining. In this context, we reasoned that systematic modification of fluorophore hydrophobicity could provide an excellent guide for future development of efficient and versatile mitochondrial fluorescent probes.

Poster Presentation : **ORGN.P-332**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Asymmetric Synthesis of β -Amino Alcohols using Acrolein Derivatives

Jae-Yeon Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

β -Amino alcohols are useful in organic synthesis and medicinal chemistry due to its biological activities such as antibacterial and anti-tuberculosis activities.¹ Recently, β -amino alcohols are used as active pharmaceutical ingredients (API) such as adrenergic agonists,² and HIV protease inhibitors.³ Generally, β -amino alcohols are good substrates for chiral ligands or chiral auxiliaries in organic synthesis.⁴ Due to its synthetic utility, development of new synthetic methods to prepare those compounds has been an active area of research.⁵ In this research, we synthesized highly optically active β -amino alcohol derivatives with good yields (up to 95%) and high enantioselectivities (up to 98% ee) from simple acrolein compounds catalyzed by chiral boron catalyst via single electron transfer mechanism.

Poster Presentation : **ORGN.P-333**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Ratiometric Two-Photon Fluorescent Probe for Monitoring of γ -Glutamyltransferase Enzyme

Jae Hyung Jo, Hwan Myung Kim*

Department of Energy Systems Research, Ajou University, Korea

γ -Glutamyltransferase (GGT) is a cell-membrane-bound enzyme, which selectively hydrolyzes the cleavage of the γ -glutamyl bond in glutathione (GSH). It is found that GGT plays an important role in cellular GSH and cysteine homeostasis, involving in diverse physiological and pathological processes. Actually, it has been discovered that overexpressed levels of GGT are connected with tumorigenesis in several human cancer cell, including ovarian and colon cancer. Therefore, GGT has been recognized as a potential biomarker of malignant tumors. In this respect, there is growing interest in fluorescent probes for GGT and several GGT activatable fluorescent probes have been developed for monitoring of GGT both in tumor cells and living animals. However, only a handful of one-photon ratiometric fluorescent probe is known that is suitable for biological imaging. In this work, we developed a new ratiometric two-photon fluorescent probe for GGT by incorporating the γ -glu-substrate and indocyanine fluorophore. This probe showed both one- and two-photon excited fluorescence and large Stokes shift as well as high cell loading ability. The probe was readily activated by GGT and successfully applied for one- and two-photon microscopy imaging in live cells.

Poster Presentation : **ORGN.P-334**

Organic Chemistry

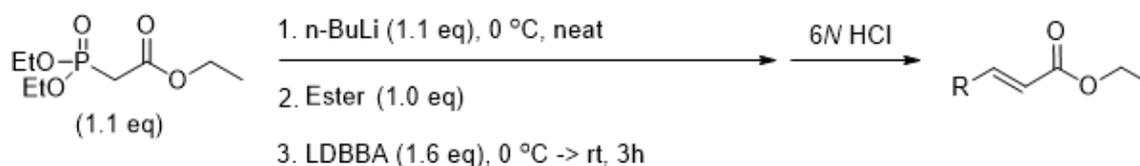
Exhibition Hall 2, THU 11:00~12:30

New method for homologation of ester to α,β -unsaturated esters using modified Horner–Wadsworth–Emmons (HWE) olefination

chang Whee Hong, Duk Keun An^{*}, Hyun Tae Kim

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 group. To the best of our knowledge, only few reports demonstrated with ester group.^{2,3} 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. Recently, we have identified reductive-HWE olefination from ester group via partial reduction followed by Wittig homologation in one pot. In continuation, the present abstract demonstrates HWE olefination with modified and efficient protocol from readily available reagents. As a result, α,β -unsaturated esters were prepared successively from the homologation of esters using LDBBA and *n*-BuLi under mild conditions (Scheme).
1. K. Kobayashi. et. al. *Tetrahedron Letters*. **2018**, 59, 568-5822. J. Jeon. et. al. *Org. Lett.* **2015**, 17, 5792-5795.3. J. Takacs. et. al. *Tetrahedron Letters*. **1986**, 27, 1257-1260



Poster Presentation : **ORGN.P-335**
Organic Chemistry
Exhibition Hall 2, THU 11:00~12:30

Targeting mitochondria and lysosome, and detect autophagy using fluorophore

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Ulsan National Institute of Science and Technology, Korea

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

Cancer is major disease of the world. Currently, most studies focus on the treatment of cancer. Preventing the occurrence of cancer is important. Autophagy prevents cancer from occurring in the early stages of cancer. In addition, it is also suppressed at the final stage of cancer development. Dysfunctional mitochondria lead to cancer and cause disease. Therefore, detection of dysfunctional mitochondria and autophagy may reduce the incidence of cancer. In addition, lysosomes play an important role in eliminating dysfunctional organelles. Therefore, it is important to target mitochondria and lysosomes separately. So, TPP_ALD is penetrated to the mitochondria with triphenylphosphonium (TPP) which is known as mitochondria targeting moiety in cancer cells and Mor_HYD is penetrated to the lysosome with morpholine which is known as lysosome targeting moiety. TPP_ALD accumulate in mitochondria and induce dysfunctional mitochondria and Mor_HYD penetrate lysosome. Subsequently, lysosome recognize the dysfunctional mitochondria and form the autophagosome. When resulted autophagosome, the TPP_ALD reacted with Mor_HYD, leading to occurrence of the blue fluorescence. That turn-on process indicate that they formed the autophagy and induce the dysfunctional mitochondria.

Poster Presentation : **ORGN.P-336**

Organic Chemistry

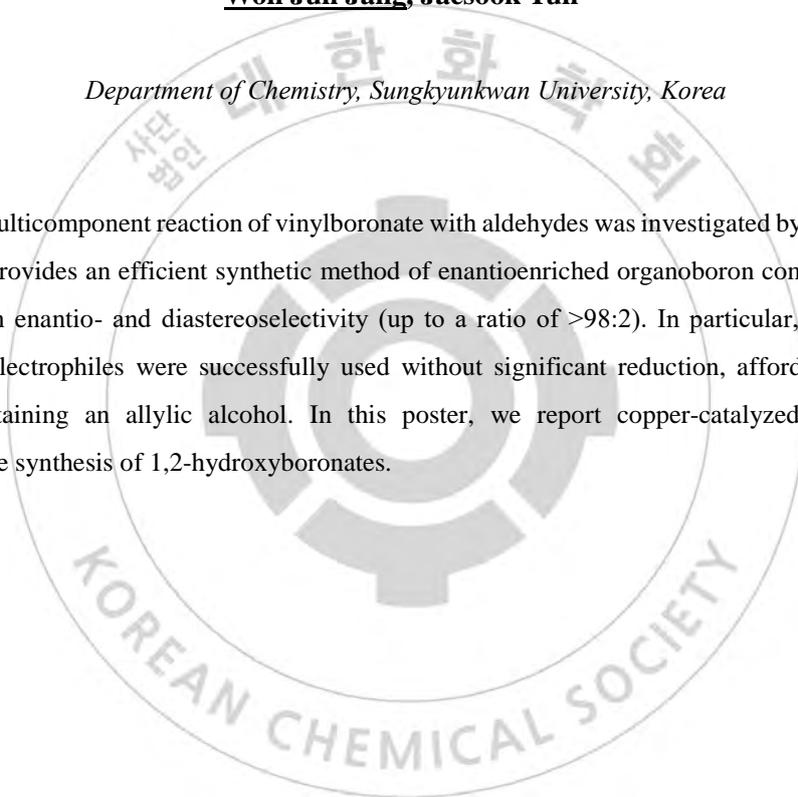
Exhibition Hall 2, THU 11:00~12:30

Copper Catalyzed Diastereo- and Enantioselective Synthesis of 1,2-Hydroxyboronates

Won Jun Jang, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Tandem and Multicomponent reaction of vinylboronate with aldehydes was investigated by Cu-H catalysis. This reaction provides an efficient synthetic method of enantioenriched organoboron compounds in good yield with high enantio- and diastereoselectivity (up to a ratio of >98:2). In particular, α,β -unsaturated aldehydes as electrophiles were successfully used without significant reduction, affording homoallylic boronates containing an allylic alcohol. In this poster, we report copper-catalyzed diastereo- and enantioselective synthesis of 1,2-hydroxyboronates.



Poster Presentation : **ORGN.P-337**

Organic Chemistry

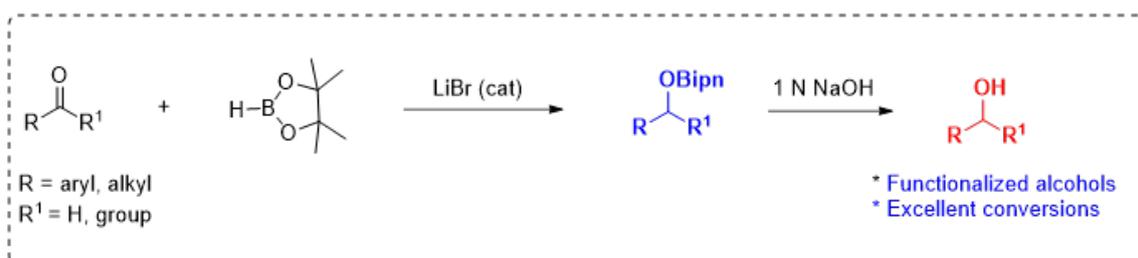
Exhibition Hall 2, THU 11:00~12:30

Novel catalytic hydroboration of aldehydes and ketones using LiBr as catalyst

Hye rim Shin, Duk Keun An*, Jea Ho Kim

Department of Chemistry, Kangwon National University, Korea

Reductions are fundamental and most frequently used chemical transformations in organic chemistry. Preparation of alcohols from reduction of aldehydes and ketones is a well-known reaction. Among the several methods for this transformation, hydride reductions are prominent in terms of yields and selectivities. Under hydride reductions, hydroboration is also an important method for the preparation of functionalized alcohols. In this regard various metal systems were reported to make this reaction more efficient with sustainable conditions. Recently, numerous catalytic systems including transition, main group, and lanthanide complexes have been reported for the hydroboration of carbonyl and unsaturated hydrocarbons.¹ However, some of these metal complexes are toxic, sensitive, expensive and requires tedious preparation of ligands. In order to overcome these issues, research is focusing on alternative catalytic systems using commercially available simple reagents for the economic and environmental concern.² As a result, we have identified and reported selective hydroboration of aldehydes and ketones with readily available sodium hydride as catalysts.³ In continuation, here we would like to present our recent experimental results for the efficient hydroboration of aldehydes and ketones with pinacolborane using LiBr as catalyst (Scheme).¹ Chong, C. C.; Kinjo, R. *ACS Catal.* **2015**, *5*, 3238– 3259. ² Wu, Y.; Shan, C.; Ying, J.; Su, J.; Zhu, J.; Liu, L. L.; Zhao, Y. *Green Chem.*, **2017**, *19*, 4169-4175. ³ Shin, W. K.; Kim, H.; An, D. K. *Tetrahedron.* **2018**, *74*, 6310-6315



Poster Presentation : **ORGN.P-338**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Enantioselective Strecker reaction of Aldimines Activated by Chiral Oxazaborolidinium Ion with Trimethylsilyl Cyanide

Sang Hyun Park, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Enantioselective Strecker reaction is useful method in synthesizing chiral α -aminonitriles which are important building blocks for many natural products¹. Various studies of nucleophilic addition to aldehydes or ketones in presence of chiral oxazaborolidinium ion(COBI) as Lewis acid catalyst have been previously reported by our group². In this research, various aldimine compounds are catalyzed by chiral oxazaborolidinium ion for the enantioselective Strecker reaction. Three-component asymmetric process studied here significantly improves upon the original Strecker reaction to obtain excellent yield (up to 98%) and high enantioselectivity (up to 95%).References¹. Miyagawa S.; Yoshimura K.; Yamazaki Y.; Takamatsu N.; Kuraishi T.; Aiba S.; Tokunaga Y.;Kawasaki T. *Angew. Chem. Int. Ed.* 2017, 56, 1055-1058.2. for selected reviews of enantioselective nucleophilic addition to aldehydes and ketones using COBI, see:(a) Kang, B. C.; Nam, D. G.; Ryu, D. H. *Org. Lett.* 2015, 17, 4810.(b) Kang, B. C.; Shin, S. H.; Yun, J.; Ryu, D. H. *Org. Lett.* 2017, 19, 6316.

Poster Presentation : **ORGN.P-339**

Organic Chemistry

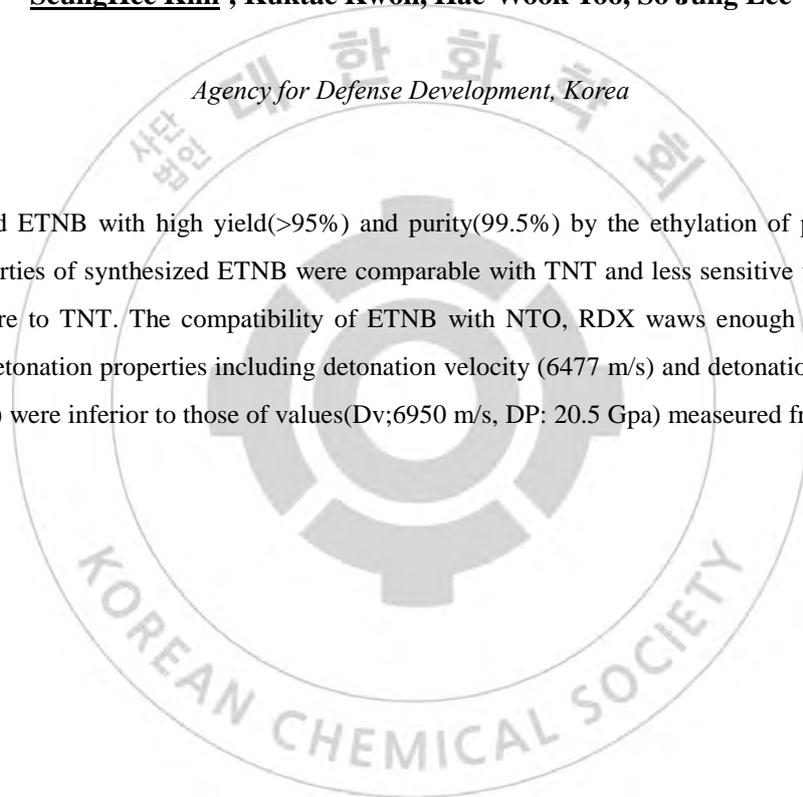
Exhibition Hall 2, THU 11:00~12:30

synthesis and characterization of ETNB(1-Ethoxy-2,4,6-trinitrobenzene) and its melt-cast formulation

SeungHee Kim*, Kuktae Kwon, Hae-Wook Yoo, So Jung Lee

Agency for Defense Development, Korea

we synthesized ETNB with high yield(>95%) and purity(99.5%) by the ethylation of picric acid. The physical properties of synthesized ETNB were comparable with TNT and less sensitive to other external stimuli compare to TNT. The compatibility of ETNB with NTO, RDX waws enough for formulation. however, its detonation properties including detonation velocity (6477 m/s) and detonation pressure (16.5 Gpa caculated) were inferior to those of values(Dv;6950 m/s, DP: 20.5 Gpa) measeured from TNT.



Poster Presentation : **ORGN.P-340**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Novel Rhodamine 6G Based Colorimetric and Fluorescent “turn-on” Chemosensor for Al³⁺

Kyoung-Lyong An, Seung Rim Shin, Kun Jun*, Sun Hye Lee¹, Soon-Jong Kim²

Korea Research Institute of Chemical Technology, Korea

¹*Mokpo National University, Korea*

²*Department of Chemistry, Mokpo National University, Korea*

A new colorimetric and fluorescent chemosensor for Al³⁺ based on Rhodamine 6G was simply synthesized and investigated for photophysical properties. Rhodamine 6G derivated fluorescent chemosensor(1) was designed and synthesized by imine synthesis of rhodamine 6G ethylenediamine and 8-Hydroxyquinoline-2-carboaldehyde. Chemosensor(1) displayed obvious color change from colorless to pink (under normal light) and non-fluorescent to yellowish-green fluorescent in the Al³⁺ direction in the acetonitrile and methylene chloride (v/v = 9:1) solution and also increased the intensity of color and fluorescence over time. And various metal ions including Ag⁺, K⁺, Li⁺, Na⁺, Ca²⁺, Cd²⁺, Co²⁺, Ni²⁺, Zn²⁺, Ba²⁺, Mg²⁺, Fe²⁺, Cs⁺, Al³⁺, Fe³⁺, Hg²⁺, Cu²⁺, Tb³⁺, Eu³⁺, Gd³⁺ caused less or smaller spectral changes. The 2:1 stoichiometry of sensor complex 1+ Al³⁺ was confirmed by Job's plot based on fluorescence emission titration. Keywords: Rhodamine 6G, Aluminium, Fluorescent, chemosensor

Poster Presentation : **ORGN.P-341**

Organic Chemistry

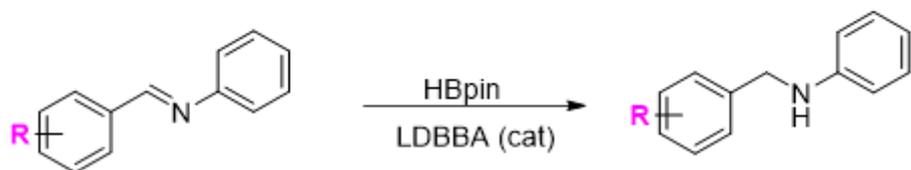
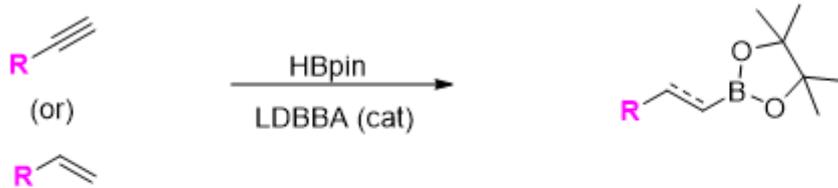
Exhibition Hall 2, THU 11:00~12:30

LDBBA catalyzed hydroboration of unsaturated hydrocarbons and imines with pinacolborane (HBpin)

Ashok Kumar Jaladi, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Hydroboration is an important and fundamental reaction system in organic chemistry. Hydroboration of unsaturated hydrocarbons such alkynes, alkenes is an effective and straight-forward method for the preparation of alkene and alkyl boronates which are versatile building blocks in various chemical transformations and metal mediated cross-coupling reactions.¹⁻² 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, 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. Therefore, efficient and sustainable method with lower active reductants are needed. During the course of our search for efficient reductions; we have identified and reported selective hydroboration of aldehydes and ketones with pinacolborane and commercial reagents as catalysts.³⁻⁴ In continuation, the present abstract demonstrates that LDBBA catalyzed hydroboration of unsaturated hydrocarbons and imines (Scheme). 1. Chong, C. C.; Kinjo, R. *ACS Catal.* **2015**, *5*, 3238– 3259. 2. Obligacion, J. V.; Chirik, P. J. *Nat. Rev. Chem.* **2018**, *2*, 15-34. 3. Shin, W. K.; Kim, H.; An, D. K. *Tetrahedron.* **2018**, *74*, 6310-6315. 4. Yang, S. J.; Jaladi, A. K.; Kim, K. H.; Gundeti, S.; An, D. K. *Bull. Korean Chem. Soc.* **2019**, *40*, 34–38.



Highly efficient method
Broad substrate scope
Excellent conversions



Poster Presentation : **ORGN.P-342**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

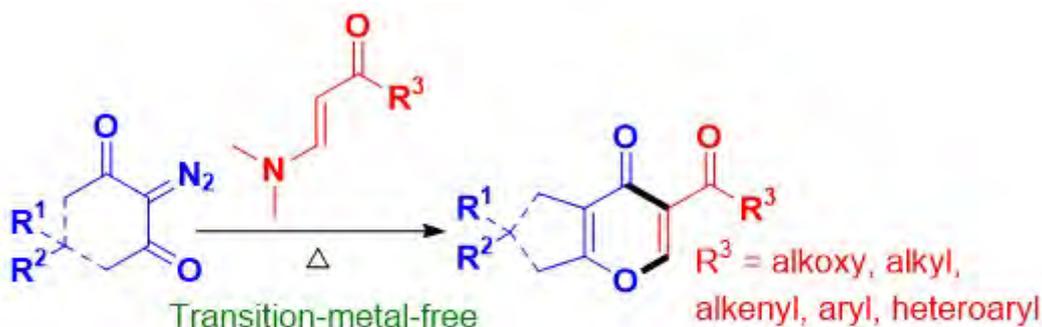
Regioselective Synthesis of Functionalized 4-Pyrones by Thermal Wolff-Rearrangement

Hyewon Kim, Yong Rok Lee^{1,*}

Chemical Engineering, Yeungnam University, Korea

¹*Division of Chemical Engineering, Yeungnam University, Korea*

4-Pyrones (γ -Pyrones) are important oxygenated heterocyclic compounds that are found widely in nature. Various 4-pyrones are known to possess biological activities, acting as anticancer, antifungal, antibacterial, insecticidal, and immunosuppressive agents. Hence, members of this class have been evaluated and utilized as drug molecules. These compounds have been also used as valuable building blocks for the construction of bioactive natural products. Owing to their importance and usefulness, various methods have been demonstrated for their construction. Although a number of methods for the synthesis of substituted 4-pyrones have been reported, more facile and efficient protocols are still highly desirable. In our continued efforts to develop new synthetic methodologies based on the Wolff rearrangement, we have been investigating transition-metal-free thermal cascade reactions of diazodicarbonyl compounds and β -enamino esters or β -enamino ketones. Herein, we report on a novel and direct regioselective construction of diverse 3-carbonyl functionalized 4-pyrones via thermal Wolff-rearrangement of diazodicarbonyl compounds.



Scheme 1. Synthetic strategy for 3-carbonyl functionalized 4-pyrones.

Poster Presentation : **ORGN.P-343**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

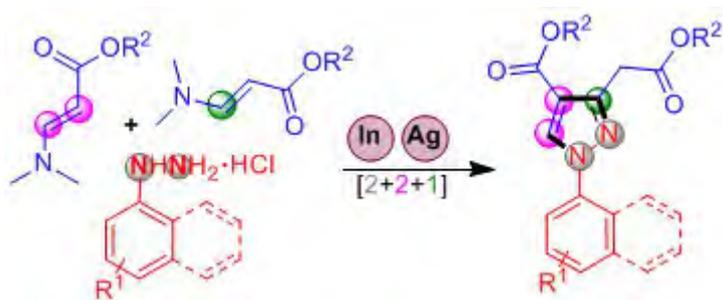
In/Ag-Catalyzed Construction of Polyfunctionalized N-Arylpyrazoles via Regioselective [2+2+1]-Oxidative N-Annulation

Raju Sitaram Thombal, Yong Rok Lee^{1,*}

Chemical Engineering, Yeungnam University, India

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Pyrazoles are among the most significant heteroaromatic compounds widely found in biologically and pharmacologically active molecules. They exhibit a variety of biological properties, including anti-inflammatory, antibacterial, analgesic, antifungal, antipyretic, antiviral, anticancer, antidiabetic, antiobesity, and plant growth regulating activities, as well as protein kinase, Cox-2, and HIV-1 reverse transcriptase inhibitory functions. They have been used as valuable building blocks and structural moifs in the synthesis of natural products, agrochemicals, dyes, and medicines. Typical approaches towards the synthesis of pyrazoles are based on the reaction of hydrazine's with 1,3-dicarbonyl compounds or unsaturated hydrocarbons by condensation and oxidation sequence, the reaction of aryl amines with 1, 3-dicarbonyl compounds forming β - amino α,β -enoates or enones, which would react further with nitriles. Accordingly, there is a demand for a facile one-step approach for the synthesis of pyrazoles. Herein, we present synthesis of polysubstituted N-arylpyrazoles by oxidative [2+2+1] cycloaddition of readily available arylhydrazine hydrochlorides with β -enamino esters by using indium (III)/ silver (I) dual catalysis (Scheme 1).



Poster Presentation : **ORGN.P-344**

Organic Chemistry

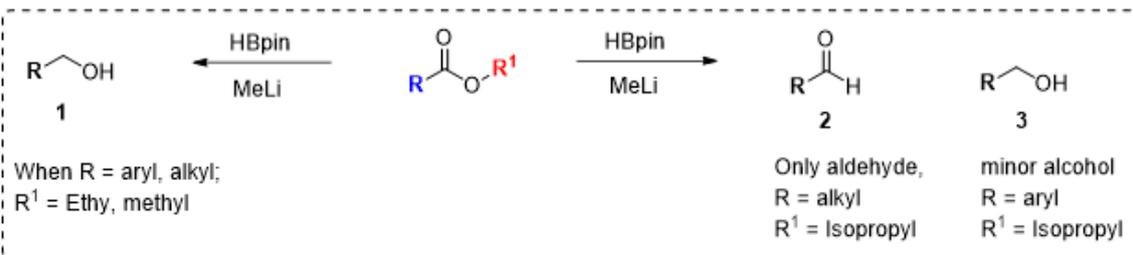
Exhibition Hall 2, THU 11:00~12:30

Partial reduction of isopropyl esters to aldehydes via catalyzed hydroboration

Ashok Kumar Jaladi, 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. In general preparation of aldehydes from esters is a two-step process (over reduction, re-oxidation). Under cryogenic conditions (-78 °C) aldehydes can be synthesized from ester group with DIBAL-H. Other than DIBAL, only few methods reported at ambient temperature. On the other hand, number of reports were described for the reduction of ester to alcohol such as metal catalyzed hydrogenation (or) hydrosilylation (or) with stoichiometric hydride addition (LiAlH₄ or LiBH₄). From our lab, we have reported convenient protocols for the aldehyde preparation via partial reduction of esters under mild reaction conditions. In recent days catalyzed hydroboration for unsaturated (C=C, C=O, and C=N) bonds became a quite rapid and hot topic in reduction chemistry as evidenced by recent publications.¹⁻² However, catalyzed hydroboration of ester are limited, and few examples are reported with Mg-based catalyst.³⁻⁴ Given our interest in the partial, selective reductions and the above situation was prompted us to carried out the catalyzed hydroboration for partial reduction of esters. Accordingly, conditions were optimized with various catalysts. Based on the experimental results, we could synthesize aldehydes from the partial reduction of isopropyl esters with pinacolborane and alkyl lithium (Scheme). 1. Chong, C. C.; Kinjo, R. *ACS Catal.* **2015**, *5*, 3238– 3259. 2. Obligacion, J. V.; Chirik, P. J. *Nat. Rev. Chem.* **2018**, *2*, 15-34. 3. Mukherjee, D.; Ellern, A.; Sadow, A. D. *Chem. Sci.*, **2014**, *5*, 959-964. 4. Mukherjee, D.; Shirase, S.; Spaniol, T. P.; Mashima, K.; Okuda, J. *Chem. Commun.*, **2016**, *52*, 13155—13158.



Poster Presentation : **ORGN.P-345**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

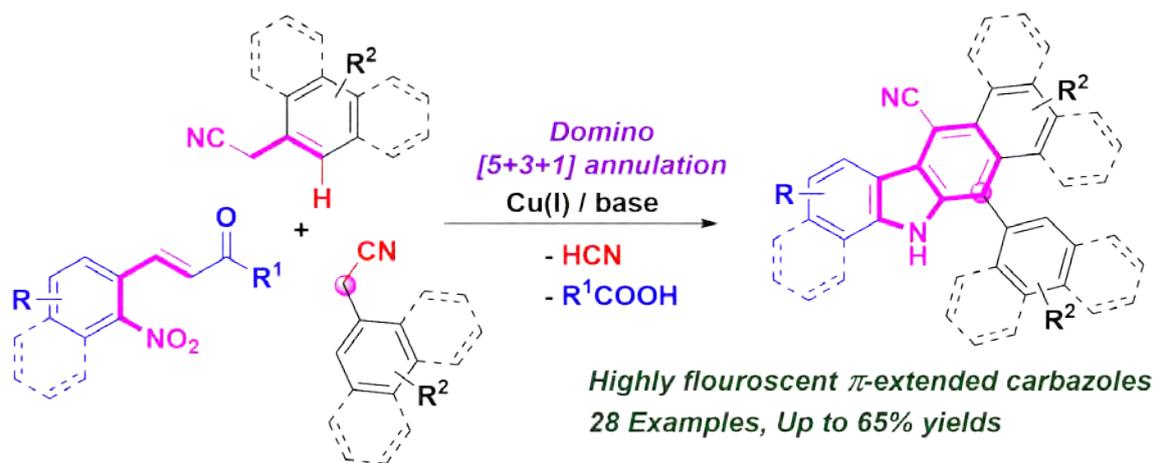
Cu(I)-Catalyzed [5+3+1] Annulation for Highly π -Extended Carbazoles

Ramuel John Tamargo, Yong Rok Lee^{1,*}

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Carbazoles and its annulated derivatives have gained widespread attention in recent years which results to their extensive biological, pharmaceutical and industrial applications. Recently, extensive efforts have been exerted to access diverse carbazoles and benzocarbazoles due to their potential anticancer, antitumor, anti-estrogenic, anti-inflammatory, and antifungal activity. Moreover, molecules bearing carbazole skeleton have been widely utilized in material science, organic light-emitting diodes, fluorescent sensors, and dye-sensitized solar cells due to its unique optical properties, high luminescent efficiency, and wide band gap. Owing to the usefulness and importance of carbazole derivatives, a number of methods for their syntheses have been developed. Despite of this, there is no report on an efficient and robust strategy to construct complex π -extended carbazole via a one-pot domino reaction using cheap and commercially available feedstock. Moreover, the effective functionalization of a versatile cyano substituent on the polyannulated carbazoles has not yet been reported. This transformation involves a sequential Michael addition/intramolecular nucleophilic addition of an enol to a nitro group/reduction of an $-\text{NO}_2$ to $-\text{NH}$ group/ intramolecular Baeyer–Villiger oxidation/carboxylic acid and HCN elimination/ 6π -electrocyclization/oxidation as supported by density functional theory (DFT) calculations. As an application, the synthesized compounds exhibited excellent fluorescence-sensing ability to detect Cu^{2+} ions. Herein, we describe the efficient synthesis of π -extended carbazole derivatives via copper-catalyzed domino [5+3+1] annulation strategy (Scheme 1).



Scheme 1. Cu(I)-Catalyzed Domino [5+3+1] Annulation Strategy for the Synthesis of Highly π -Extended Carbazoles



Poster Presentation : **ORGN.P-346**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Facile aromatic CF₃ substitution and [¹⁸F]CF₃ labeling from aryl iodides by using the Cu ligand complex [(TMPhen)₂Cu][COOCF₂Cl]

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Drugs containing trifluoromethyl group have more high lipophilicity, in vivo stability and cell permeability. For this reason, aromatic trifluoromethylation and [¹⁸F]trifluoromethylation is very useful for development of new drugs as well as PET imaging agents. In this study, we explored the various ligands to discover the efficient ligand for copper mediated trifluoromethylation of aryl iodide. To figure out the most efficient ligand, a series of σ -donor and π -donor ligands were tested and compared the reactivity for trifluoromethylation. The CF₃ substitution was performed in presence of copper iodide, methylchlorodifluoroacetate (MCDFA), potassium fluoride, ligands and 1-iodo-4-nitrobenzene as a model compound. Based on condition of the CF₃ substitution, [¹⁸F]trifluoromethylation was carried out. As results, the most efficient ligand was 3,4,7,8-tetramethylphenanthroline (TMPhen) that has the highest yields for trifluoromethylation (35.5 \pm 8.4%, $n \geq 3$) as well as [¹⁸F]CF₃ substitution (72 \pm 2.0%, $n \geq 3$) as compared with reported ligand TMEDA (4.7 \pm 0.7% and 44 \pm 5.8%, $n \geq 3$, respectively) [1]. In addition, [¹⁸F]trifluoromethylation of various aryl iodides obtained the desired products in moderate yields. The Cu ligand complex [(TMPhen)₂Cu][COOCF₂Cl] was synthesized and analyzed by single X-ray crystal and NMR. The trifluoromethylation of model compound with complex gave desired product in more high yields (85.0 \pm 1.4%). In this study, we investigated various ligands for trifluoromethylation to find the most efficient ligand. According to results, TMPhen was shown to best yields for CF₃ substitution. This methodology applied for the synthesis of various [¹⁸F]trifluoromethyl substituted arene derivatives.[1] M. Huiban, M. Tredwell, S. Mizuta, Z. Wan, X. Zhang, T. L. Collier, V. Gouverneur, J. Passchier, Nat. Chem., 2013;5:941–944.

Poster Presentation : **ORGN.P-347**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

BTC5A (Bis-Triethylene glycol-functionalized Crown-5-calix[4]Arene) analogs as a new phase-transfer catalysts for nucleophilic aromatic [¹⁸F]fluorination

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Aromatic fluorine-18 labeling into the bioactive molecule is essential for in vivo stability and retaining its biological activities as PET radiotracers. As the above reason, new effective incorporation of fluorine-18 into arene is always in demand. Herein, we intend to achieve an effective aromatic [¹⁸F]fluorination in various conditions by using BTC5A analogs as a new phase transfer catalyst. We evaluated the reactivity of six differently substituted biphenyl precursors and chosen diaryliodonium salt precursors as the desirable precursor. In the stability test of precursors with PTC in basic conditions showed up to 30% higher stability in case of BTC5A analogs compare to Kryptofix2.2.2 (K_{2.2.2}). When using TEMPO as radical scavenger with PTC, showed that precursor was more stable in basic conditions. After the stability test, aromatic fluorination from the precursor by using KF with BTC5A analogs were performed in the optimized condition and showed that highest yields up to 80% which is about 10 times higher than K_{2.2.2}. In fluorine-18 labeling experiments, the radiochemical yield (RCY) in the presence of BTC5A analogs & TEMPO showed up to 82% which is three times higher than that in the presence of using K_{2.2.2}. We also found that RCY was about 40% even though only 10 mole% of BTC5A analogs was used. In this study, we could successfully optimize the condition for the F-18 labeling by using BTC5A analogs which is more effective than K_{2.2.2}. We are expecting that BTC5A analogs as an organic promoter could be an alternative catalyst for aromatic [¹⁸F]fluorination and also help to develop new radiopharmaceuticals.[1] Dong Wook Kim, et al. Chem. Eur. J. 2016, 22, 4515-1520[2] Byung Chul Lee, et al. Org. Biomol. Chem. 2011, 9, 8346-8355

Poster Presentation : **ORGN.P-348**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

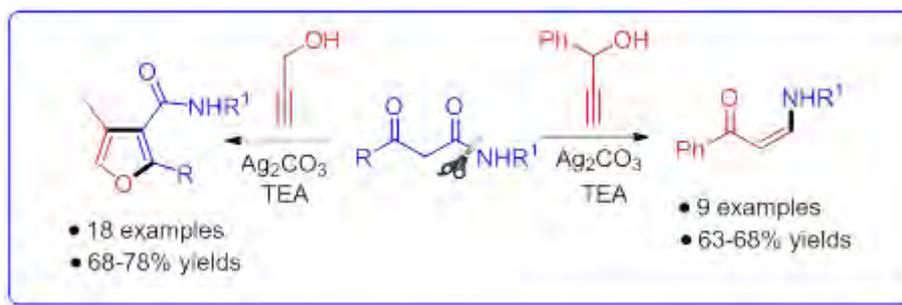
Ag(I)-Mediated Regio- or Stereoselective Synthesis of Furan-3-carboxamides and (Z)-Enaminones

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Furans bearing amide groups have been recognized as important subunits in many biologically active molecules, especially in agrochemicals. Owing to the importance of furan rings, several synthetic approaches have been reported, however synthetic approaches to amide substituted furan rings have been less explored so far. Among these, the typical method for furan-3-carboxamides involves by multi-step reactions and preparation of starting materials. Enaminones show a versatile reactivity in organic synthesis and are important building blocks for the synthesis of biologically interesting heterocycles and aromatic compounds. Over the past decade, a number of methods have been developed for the preparation of (E)- and (Z)-enaminones. However, a more facile and efficient one-pot synthetic protocol is still desirable. This demanded the development of one-pot reaction from easily readily available starting materials. So, we were encouraged to develop a new synthetic one-pot methodology for the construction of furan-3-carboxamides by using commercially available β -oxo amides and propargyl alcohol mediated by silver carbonate. The important feature of this process is the reaction is regioselective and controlled by propargyl alcohol. With employing a substituted propargyl alcohol, highly stereoselective (Z)-enaminones have been obtained.



Poster Presentation : **ORGN.P-349**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Mild Base Mediated Benzannulation of N-Tosylhydrazones with 3-Formylchromones: Direct Access to Diverse and Polyfunctionalized Xanthenes

Rajeev Shrestha, Yong Rok Lee*

Division of Chemical Engineering, Yeungnam University, Nepal

N-tosylhydrazones have been paid more attention in organic chemistry as a precursor or sources of diazo compounds. A number of transition-metal-catalyzed and transition-metal-free transformations of *N*-tosylhydrazones via cyclopropanation, C–H insertion, ring expansion, coupling reactions, and construction of heterocycles have been demonstrated. Despite remarkable and excellent developments of novel mythologies using *N*-tosylhydrazones in organic synthesis, there are no reports on the reactions of *N*-tosylhydrazones with 3-formylchromones so far. In this context, the reaction of *N*-tosylhydrazones with 3-formylchromones in the presence of base was examined leading to unexpected xanthenes. Xanthenes are important oxygenated heterocycles found in many natural products exhibiting prominent biological and pharmacological activities. Especially, xanthenes moiety exhibit potent anticancer, antimicrobial, antimalarial, anti-HIV, antioxidant, antialzheimer, protein kinase C, α -glucosidase, and cholesterol acyltransferase inhibitory activities. Moreover, some of these compounds are evaluated and employed as major drug candidates. Although several approaches for the synthesis of xanthenes have been well described, more facile and efficient protocols for diverse and functionalized xanthenes are still highly desirable. Herein, we present simple and efficient base-promoted denitrogenative/deoxygenative/deformylative condensation for the regiospecific construction of biologically interesting polyfunctionalized xanthenes starting from *N*-tosylhydrazones and two molecules of 3-formylchromones (Scheme 1). This protocol proceeds via a cascade diazo formation/Michael addition/denitrogenation/[4+2] cycloaddition/deformylation/ring opening. The synthesized compounds showed potent UV-filter properties compared to common sunscreen agents, excellent turn-off fluorescence sensing properties for Fe³⁺ ions, and antioxidant activities comparable to standard BHT.



Poster Presentation : **ORGN.P-350**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Ratiometric detection for indium ions using fluorescent probes consisting of aggregation induced emission fluorophore and dipeptide receptor

Joohee Park, Chaeun Kim, Keun Hyeung Lee*

Department of Chemistry, Inha University, Korea

Indium is widely used in the manufacturing of semiconductor, solar cell, and industrial products, however, it is one of the most scarce metal ions. Considering the increased demand of indium in the recycling process and in the production from ores, the cheap, easy, and real-time monitoring methods to detect indium have been demanded. A fluorescent probe (1) for trivalent ions was synthesized based on the dipeptide receptor and aggregation induced emission(AIE) and twisted internal charge transfer process. 1 showed a more selective ratiometric response to In (III) than Al (III) and Ga (III) at pH ranged from 5.0 to 5.5. Upon adding Indium ions, 1 showed ratiometric emission changes with significant increase of the emission at 600 nm and decrease of the emission at 540 nm with the excitation of 470 nm. 1 with high metal binding affinity ($3.34 \times 10^6 \text{ M}^{-1}$) showed highly sensitive ratiometric response to In(III) ions and detection limit for In (III) ions is 490 nM in aqueous buffered solution. The binding mode study of 1 with In (III) ions was carried out using Job's plot analysis, pH titration experiments, NMR, FT-IR, Mass complex, and DLS measurements.

Poster Presentation : **ORGN.P-351**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Highly Selective and Sensitive Detection of Heparin based on A Self-Assembled Conjugated Polyelectrolyte Micelle

Yeonjin Jang, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

This study, we demonstrated that a self-assembled conjugated polyelectrolyte micelle (CPM) induces very sensitive signal transduction involving amplified fluorescent changes, which marks a strong difference with the numerous fluorescence-based assays 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 the hydrophilic functionality 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 CPM drives highly selective and sensitive detection of heparin at very low concentrations.

Poster Presentation : **ORGN.P-352**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Study on the Reaction Property of Copper(I)-catalyzed Azide-Alkyne Cycloaddition(CuAAC) Click Reaction Using Fluorescent Peptide

Jaewook Jeong, You Hyeongseok, Keun Hyeung Lee*

Department of Chemistry, Inha University, Korea

CuAAC click reaction was well-known to transform 1,4-triazole between alkyne and azide. In this study, we synthesized a fluorescent peptide(**1**) for monitoring intramolecular CuAAC click reaction in 50% aqueous solution containing two pyrene fluorophores. Upon addition of Cu(II) in the presence of ascorbic acid, intramolecular CuAAC click reaction of the probe occurred, resulting in the enhancement of monomer emission and decrease of excimer emission. As the concentration of Cu(II) increased from 1 to 5 equivalent, the rate of click reaction increased. We investigated the rate of CuAAC click reaction controlled by Cu(II) pH effect, buffer effect and other catalysts(additives, etc) of this reaction.

Poster Presentation : **ORGN.P-353**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Conjugated Polyelectrolyte Micelle-Based Fluorescent pH Sensors for Strongly Acidic or Basic Conditions

Jeongmoo Lee, Seung Ho Lee*

Department of Chemistry, Daegu University, Korea

In this work, effective fluorescent pH sensors have been developed for extreme acidic or basic conditions 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 monomers display the self-assembled micelle formation in extreme acid or base range of pH, giving the hydrophobic π -extended conjugated system at the inner part and hydrophilic functionality 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 extreme pH conditions.

Poster Presentation : **ORGN.P-354**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Conjugated Polyelectrolyte Micelle Based Kinetic Discrimination of Fe²⁺ and Fe³⁺

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¹*Department of chemistry, Daegu University, Korea*

²*Department of Chemistry, Daegu University, Korea*

A great effort has been gone into the discrimination of Fe²⁺ and Fe³⁺ ions due to their involvement in various environmental and biological systems. In this work, a conjugated polyelectrolyte micelle based fluorescence system has newly developed to discriminate Fe²⁺ and Fe³⁺ based on their induced quenching kinetics. A particular amphiphilic building block with a pyrene 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 functionality at the periphery. This system allows enhanced optical properties with efficient energy or electron transfer, and high fluorescence quantum yield, which permits more effective amplified quenching in conjugated system of pyrene aggregates in the presence of Fe³⁺ ion.

Poster Presentation : **ORGN.P-355**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Bio-orthogonal turn-on probe Tetrazine based Kaleidolizine

Sang-Kee Choi, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Indolizine based fluorophore Kaleidolizine(KIz) is known as tuning the emission wavelength by changing 3 positions of its substituents. The KIz can offer a clear view with ultraslow background signal because of its property of Aggregation-Induced Emission(AIE). Additionally, the well-known fluorescent quencher tetrazine is applied as the substituent of KIz to act both as reactive handle and quencher moiety. To minimize electronic interference, the tetrazine is existed on the shared π -system with short distance on R1, R2, and R3 position. Since the property of tetrazine acts as a fluorescent quenchers based on resonance energy transfer(RET). Tetrazine is having attention with its fast and chemoselective [4+2] cycloaddition with specific dienophiles such as Trans-cyclooctene(TCO) without any catalysts. With high selective 'tagging' of specific targets, it can provide a means to image or track the components and interactions. As the quenched fluorophore, the tetrazine-based KIz implies with various application methods by lowering the background signal to enhance the turn-on ratio.

Poster Presentation : **ORGN.P-356**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Rationally Designed Organocatalysts for CO₂-based Cyclic Carbonates

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Cyclic carbonates synthesized from the cycloaddition of carbon dioxide and epoxide are known to be useful compounds with many applications. To date, a wide range of catalytic systems including metal-based catalysts and organocatalysts have been developed for the coupling of CO₂ and epoxides. However, to complete this reaction, many catalysts require harsh reaction conditions such as high temperatures (> 75 °C), high CO₂ pressures (> 10 bar) and high catalyst loadings (> 5 mol %), which are ultimately associated with additional, indirect CO₂ emissions and limit their value from a technological standpoint. Only few examples of organocatalysts for the synthesis of cyclic carbonates via the coupling of CO₂ and epoxides under the mild condition of room temperature have been reported in the literature. We will report novel bifunctional one-component organocatalysts that resemble scorpions effectively couple carbon dioxide and epoxides under room temperature, low-catalyst-loading (2 mol%), low-carbon-dioxide-pressure (1–10 bar), and solvent-free conditions.

Poster Presentation : **ORGN.P-357**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

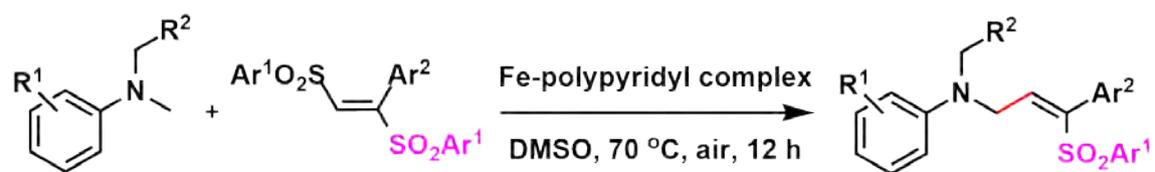
Iron-polypyridyl Catalyzed Oxidative Alkenylation of Tertiary Aniline with Vinyl Sulfone

Sanghyeok Lee, Joon Young Hwang, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

The direct alkenylation reaction of an α -amino C(sp³)-H bond of tertiary aniline with (*E*)-1,2-bis(arylsulfonyl)ethylene was achieved using iron-polypyridyl complex. Photoredox radical alkenylation of α -amino acids and *N*-aryl amines was investigated by MacMillan using Ir(III) catalyst, and Inoue also reported the related protocol employing benzophenone under metal-free and photo-irradiation condition.¹ In the context of an increasing interest in iron redox catalysis, oxidative transformation of amines by iron catalysts have been mostly limited in the iminium formation due to the uncontrollable oxidative property.² As a mild single-electron-transfer (SET) oxidation condition for the formation of α -aminoalkyl radical species, polypyridyl ligands were introduced to iron salts, based on electron donating effect of ligand to metal center. Iron-polypyridyl complex successfully generated the nucleophilic α -aminoalkyl radical species, which was reactive to (*E*)-1,2-bis(arylsulfonyl)ethylene as electron-deficient alkene. After α -aminoalkyl radical is trapped vinyl sulfone, elimination of β -sulfonyl radical would provide the allyl amine product. The derived allyl amine products containing a sulfonyl group were further converted in a single step to the pyrrole derivatives *via* cyclization and aromatization steps with ethyl isocynoacetate.^{1b}

Acknowledgement This study was supported by the Ministry of Education, Science and Technology, National Research Foundation (Grant No. 2018R1A2B6008824). **Reference** (1) (a) Noble, A.; MacMillan, D. W. C. *J. Am. Chem. Soc.* **2014**, *136*, 11602-11605.; (b) Amaoka, Y.; Nagatomo, M.; Watanabe, M.; Tao, K.; Kamijo, S.; Inoue, M. *Chem. Sci.* **2014**, *5*, 4339-4345 (2) (a) Kumaraswamy, G.; Murthy, A. N.; Pitchaiah, A. *J. Org. Chem.* **2010**, *75*, 3916-3919; (b) Li, Y.; Jia, F.; Li, Z. *Chem. Eur. J.* **2013**, *19*, 82-86; (c) Zhao, M-N.; Yu, L.; Hui, R-R.; Ren, Z-H.; Wang, Y-Y.; Guan, Z-H. *ACS Catal.* **2016**, *6*, 3473-3477.



Poster Presentation : **ORGN.P-358**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Core-Shell Structured P3PT-Wrapped CNT Bucky Paper

Sung-jin Kim, Ueon Sang Shin*

Nano-Bio Medical Science, Dankook University, Korea

The crucial obstacle to design an electrically conducting device is the poor and heterogeneous dispersion of the pristine CNTs in polymer matrices. The best method to overcome these problems is to create a CNT-core-polymer shell structure, allowing a dense close-packing of the CNT core-polymer shell units, expecting in the formation of completely homogeneous CNT-polymer films and a big improvement in their physicochemical properties including the electrical conductivity. Poly[3-(5-carboxypentyl)thiophene-2,5-diyl] wrapped multi-walled carbon nanotubes (P3PT-COOH/CNTs) in core-shell structure were successfully prepared as a bucky paper by simple pH-control of the aqueous solution containing different weight percentages of the both components (P3PT-COOH/CNTs = 50/50, 60/40, 70/30). The core-shell structure of P3PT-COOH/CNT-50 nanohybrid films showed a significantly high electrical conductivity increase of up to 17 fold compared with those of non-core-shell structure prepared by a simple mixing (e.g. from 1.33 to 1.81 S/cm up to 22 S/cm). The result could be considered to be a consequence of a homogeneous P3PT-COOH-wrapping on the surface of CNTs, the regular shell thickness of individual CNT-core/P3PT-COOH-shell nanohybrid fibers, and their three-dimensional close packing in a film.

Poster Presentation : **ORGN.P-359**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Selective red-emission detection of Glu in aqueous solution at physiological pH using fluorescent probe based on phenylboronic acid and amphiphilic peptide receptor

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¹*Department of Chemistry, Inha University, Korea*

Glucose is the principal source of energy production for important organs in humans. Metabolic defects in glucose and energy metabolism causes several health problems including diabetes mellitus. We reported a fluorescent peptidyl probe (1) based on the dipeptide containing boronic acid and twisted internal charge transfer (TICT)-active fluorophore, cyanostilbene. The probe showed selective detection of Glu among sugars in aqueous solution at physiological pH and basic pH (7.4~11.5) by a red-emission response. The probe (1) did not aggregate in aqueous solution, exhibiting a significant emission at 535 nm. Upon addition of Glu, the probe aggregated and formed nanoparticles, showing significant enhancement of the emission at 600 nm with concomitant decrease of emission at 535 nm, as revealed by fluorescence, dynamic light scattering, and transmission electron microscopy studies. The binding mode study suggested that the probe may formed a 2:1 adduct with Glu, resulting in the aggregation of the adduct and the probe formed a 1:1 adduct with fructose that did not aggregate.

Poster Presentation : **ORGN.P-360**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

An injectable hydrogel preparation for sustained Cyclosporin A delivery

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¹*Nano-Bio Medical Science, Dankook University, Korea*

Cyclosporine A (CsA) is an extremely hydrophobic immunosuppressive drug, whose systemic administration to suppress the activity of T cells and T cell-based immune responses is frequently associated with a number of adverse drug reactions. Local delivery of CsA focused on a specific target organ has been proposed as a possible solution to this problem. In this study, we developed biodegradable sol-gel drug delivery systems, consisting of HA-Ca-Alg hydrogels combining hyaluronic acid calcium complex (HA-Ca) and sodium alginate (Alg-Na) components, for the local sustained delivery of CsA. A HA-Ca complex with very high degree of substitution was prepared by the acid-base reaction of hyaluronic acid and calcium acetate. The gelation was completed within about 2–45 min without external addition of salts, indicating the high potential of the present hydrogel systems for drug delivery by injection in vivo. The HA-Ca system was characterized by several analysis methods. Moreover, the scanning electron microscopy analysis of the HA-Ca-Alg hydrogels showed an irregular porous morphology, with interconnected pores of 50–300 μm width. The sol-gel transition and the maximum viscosity (about 10,000 cP) of the HA-Ca-Alg hydrogels were characterized by examining the time evolution of the viscosity at 37 C. The hydrolytic degradation of the HA-Ca-Alg hydrogel was also examined at 37 C. CsA-encapsulated HA-Ca-Alg hydrogels exhibited sustained in vitro release of CsA over 14 days, which was confirmed through in vitro measurements of the activity of murine T cells over 2 weeks. These results show that the present injectable HA-Ca-Alg hydrogels can be used effectively for the sustained delivery of extremely hydrophobic immunosuppressive drugs, including CsA.

Poster Presentation : **ORGN.P-361**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

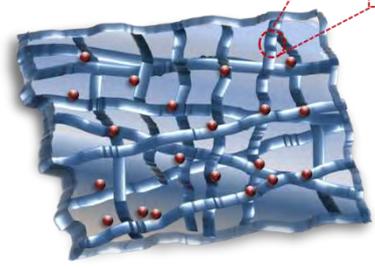
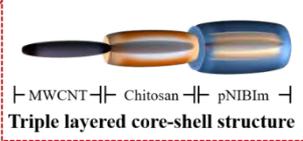
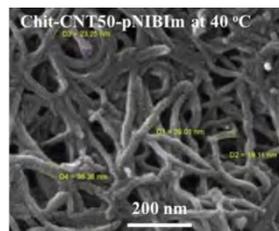
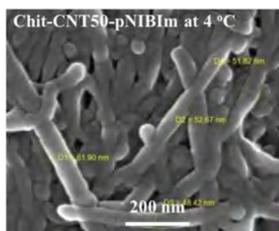
Carbon Nanotube-Based Smart Transdermal Drug Delivery System (TDDS)

Ji-Hye Kang, Ueon Sang Shin^{1,*}

Department of Nano-Bio Medical Science, Dankook University, Korea

¹Nano-Bio Medical Science, Dankook University, Korea

Smart carbon nanotube-framed (SCNF) membranes were prepared by self-assembly of highly thermo conductive CNT molecules hybridized with chitosan (Chit) in a core-shell structure and then by chemical integration of a temperature-responsive copolymer, poly(NIPAAm-co-BVIm) (or pNIBIm), as an additional outer shell. The SCNF membranes had a three-dimensional interwoven porous nanostructure. CNT, Chit, and pNIBIm components used in the SCNF membranes function as a thermally conductive CNT-framework, a biocompatible glue to stick the CNT building blocks together, and a temperature-responsive copolymer, respectively. The SCNF membranes with different Chit/CNT ratios and an almost constant pNIBIm concentration (Chit-CNT25-pNIBIm, Chit-CNT50-pNIBIm and Chit-CNT75-pNIBIm) had a three-dimensional interwoven porous nanostructure. Scanning electron microscopy clearly showed the temperature-responsive swelling and deswelling characteristics of the triple core-shell structured CNT-frames. Temperature-dependent bovine serum albumin (BSA)-loading and -release profiles were obtained at 4 °C, 25 °C, 36.5 °C, and 40 °C. Especially the Chit-CNT50-pNIBIm hybrid membrane showed a markedly high loading capacity of 9.7 mg per mg of membrane at 4 °C. It also showed a temperature-dependent BSA-release characteristic (0.92 mg/mg at 36.5 °C and 3.41 mg/mg at 40 °C). The SCNF membranes showing highly effective drug-loading/-releasing characteristics could be potentially used as a skin heat signal-responsive patch type transdermal drug delivery system (TDDS) in the medicinal field.



~ LCST (37-40°C)
Skin heat signal
<< LCST (4-25°C)



Transdermal drug delivery



Poster Presentation : **ORGN.P-362**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Aluminum amide mediated conversion of amides into amidines: Synthesis of amidine library

Sang-Hyeup Lee

Department of Life Chemistry, Daegu Catholic University, Korea

Amidines are the valuable precursors for the synthesis of a wide variety of heterocyclic ring systems such as quinazolines, imidazoles, pyrimidines, and triazoles etc. They are representing an important pharmacophore in drug discovery and have been indicated as potential agents for the treatment of Alzheimer's disease, malaria, and as inhibitors of acid-sensing ion-channels, platelet aggregation and serine protease. In addition, they have employed in the field of material science, catalyst design and also shown its capacity to fix carbon dioxide. Accordingly, a number of synthetic methods have been reported for the preparation of amidines. The most of the methods involve disconnection of the product to an iminium cation synthon and a nitrogen nucleophile. Unlike primary and secondary amides, till now, tertiary amides has not been utilized as starting materials in the synthesis of N,N,N'-tri substituted amidines. This approach was extended to the four folds diversity oriented synthesis of N,N,N'-tri substituted amidines using various building blocks. Furthermore, it is a convenient method to access N-mono, N,N disubstituted, N,N'-substituted amidines, N,N,N'-tri substituted amidines in good yields by the reaction of primary, secondary and tertiary amides with dimethyl aluminum amide reagents derived from various typical classes of primary and secondary amines and AlMe₃.

Poster Presentation : **ORGN.P-363**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of 2-alkoxybenzimidazoles and its conversion into 2-aminobenzimidazoles using aluminum amides

Sang-Hyeup Lee

Department of Life Chemistry, Daegu Catholic University, Korea

Aminobenzimidazole is an important structural unit in medical chemistry, due to its wide a range of biological activities which comprises nearly one-quarter of the top 100 so called known drugs such as Vermox, Fenbendazole, oncadazole, and mizalastine. Particularly, 2-Aminobenzimidazole core is found in antagonists against glucagon receptor, G9a histone methyltransferase, 1L-1 receptor-associated kinase-48, inducible T-cell kinase, and H3-receptor. To the best of our knowledge, there is no report for the preparation of 2-alkoxy & 2-aminobenzimidazoles using azidoanilines. Even there are so many procedures were documented for the preparation of that substrates. In continuation of this work, we are developing Synthesis of a library of 2-Aminobenzimidazole is described. In this approach, an array of 2-alkoxybenzimidazoles was synthesized using coupling reaction between various chloroformates and azidoanilines, N-alkylation and cyclization via Staudinger reaction followed by aza-wittig reaction. These substrates were finally treated with under smart diversity-building cleavage conditions using a series of aluminum amide complexes to afford the corresponding 2-Aminobenzoxazole products in excellent yields and purity.

Poster Presentation : **ORGN.P-364**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Dibenzothiophene based material for non-doped fluorescent emitter and Yellow phosphorescent organic light emitting diodes

Kyu Yun Chai*, **Braveenth Ramanaskanda**, **Sohyeon Kim¹**, **Hasu Jung²**, **Subin Oh¹**

Department of Chemistry, Wonkwang University, Korea

¹*Wonkwang University, Korea*

²*Organic Chemistry, Wonkwang University, Korea*

New bipolar material DBTO-IN/ CAR (2-(5-phenylindolo[3,2-a]carbazol-12(5H)-yl)dibenzothiophene 5,5-dioxide) was designed and synthesized. The material showed excellent glass transition temperature of 156 °C, which manifests as a high thermal stability of DBTO-IN/CAR. We have constructed two different devices, namely a non-doped bipolar fluorescent emitter a green phosphorescent OLED with DBTO-IN/CAR bipolar material. The DBTO-IN/CAR host material-based device showed excellent maximum current and power efficiencies of 51.98 cd/A and 45.36 lm/W, respectively. The reference CBP-based similar device exhibited a lower power efficiency of 42.01 lm/W. The DBTO-IN/CAR-based host device revealed a good external quantum efficiency of 19.03%. Consequently, the non-doped DBTO-IN/CAR fluorescent emitter related device also exhibited better current and external quantum efficiencies of 4.30 cd/A and 2.47%, respectively, with the CIE of 0.23, 0.41.

Poster Presentation : **ORGN.P-365**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Dibenzo carbazole based host materials for Yellow phosphorescent organic light emitting diodes

Kyu Yun Chai*, **Seung Yu Choi¹**, **Keunhwa Kim¹**, **Keunhwa Kim¹**, **Youngee Park¹**

Department of Chemistry, Wonkwang University, Korea

¹*Wonkwang University, Korea*

Two host materials, 7-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-7H-dibenzo[a,g]carbazole (TRZ-DBC1 and TRZ-DBC2) were designed and synthesized. The both materials showed excellent thermal stabilities with good bipolar characteristics. In order to understand the device efficiencies, we have fabricated yellow phosphorescent OLED devices with reference CBP material. The TRZ-DBC1 based yellow device exhibited excellent current efficiency of 71.4 cd/A, while reference device revealed lower efficiency of 58.0 cd/A. The lower turn on voltage of 2.3 and 2.5 V were noticed for TRZ-DBC1 and TRZ-DBC2, respectively. The external quantum efficiency of TRZ-DBC1 (25.4%) and TRZ-DBC2 (22.4%) were excellent when compare to reference CBP based device (19.1%). TRZ-DBC1 and TRZ-DBC2 based yellow devices showed excellent luminescence of 65,660 cd/m² and 98,680 cd/m², respectively. These two bipolar host materials would be promising candidates for yellow phosphorescent OLEDs for display application

Poster Presentation : **ORGN.P-366**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

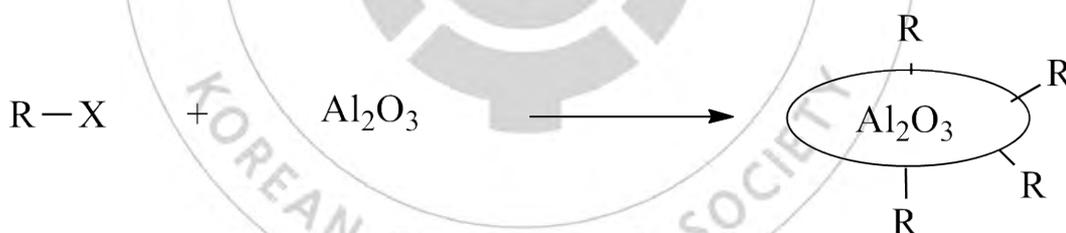
Organic Functionalization of Porous Alumina: Luminescence Properties

Yongcheol Jung, Chuljin Ahn^{1,*}

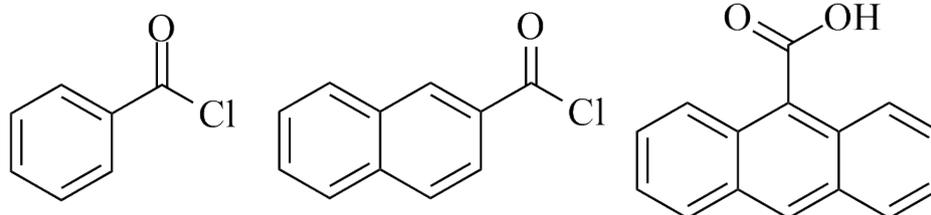
Department of Chemistry, Changwon National University, Korea

¹*Department of Biology and 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.



R-X :



Poster Presentation : **ORGN.P-367**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

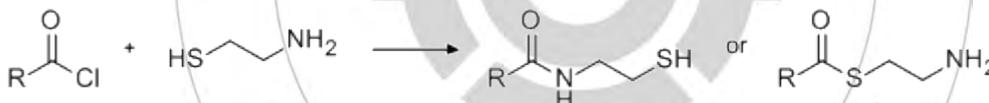
The Investigation of Chemoselectivity in β -mercaptoamine Depending on Reaction Condition: S-Acylation vs N-Acylation

Myeonghwan Shin, Chuljin Ahn^{1,*}

Department of biology and chemistry, Changwon National University, Korea

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

The chemoselectivity is important to control functionalization in a molecule. In this research, we investigated the selectivity between S-acylation and N-acylation depending on reaction condition with β -mercaptoamine and acid chloride.



Poster Presentation : **ORGN.P-368**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

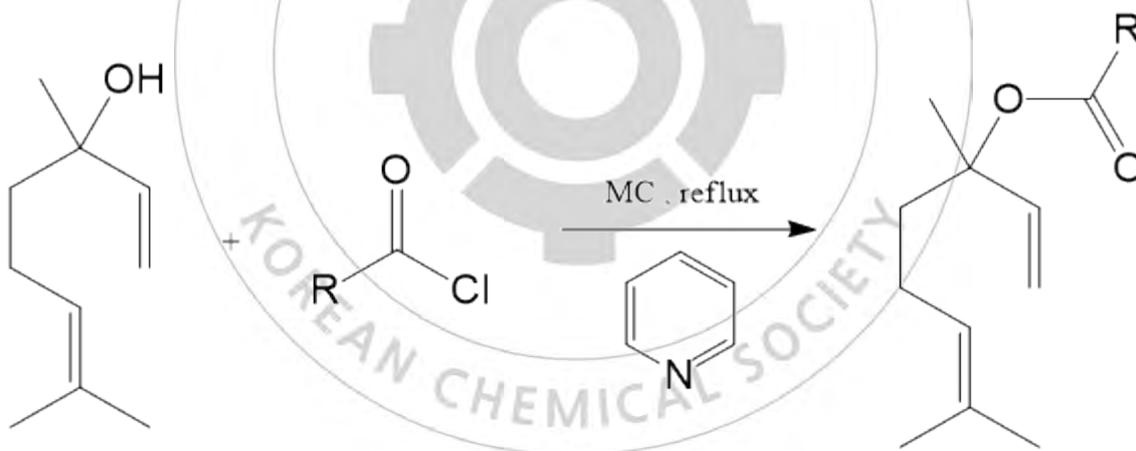
Preparation of Linalool Derivatives; Their Fragrance and Application

JiEun Lee, Chuljin Ahn^{1,*}

Changwon National University, Korea

¹*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 were investigated their fragrance.



Poster Presentation : **ORGN.P-369**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Mono and bridged BODIPYs: their synthesis, structures and spectroscopic properties

Galam Jung, Seungoh Hong, Se Won Bae*

Green Chemistry & Materials Group, Korea Institute of Industrial Technology, Korea

Covalently linked pairs of chromophores have been a matter of interest for the scientific community for a long time. Such chromophore dimers have been found in biology, for example, photosynthetic bacterial proteins and natural light harvesting antenna systems. Numerous artificial fluorescent dyes have been used in biosciences for cell imaging and investigation of in vivo biological processes. The boron dipyrromethenes (BODIPYs) are a well-known class of highly emissive molecules and they have been found to be extremely useful for biological applications, e.g. biochemical labelling, photosensitizers for PDT (Photo Dynamic Therapy) and fluorescent probes. The electronic and photophysical properties of BODIPYs can be fine-tuned for different applications by the structural modification of the boron-dipyrrin core or by making their dimers and oligomers. Reports on covalently linked BODIPY dimers are on the rise but still there is a need to study the photophysical properties of mono and bridged BODIPY dimers. In this contribution, we present the synthesis, structures and photophysical properties of mono and bridged BODIPY dimers.

Poster Presentation : **ORGN.P-370**

Organic Chemistry

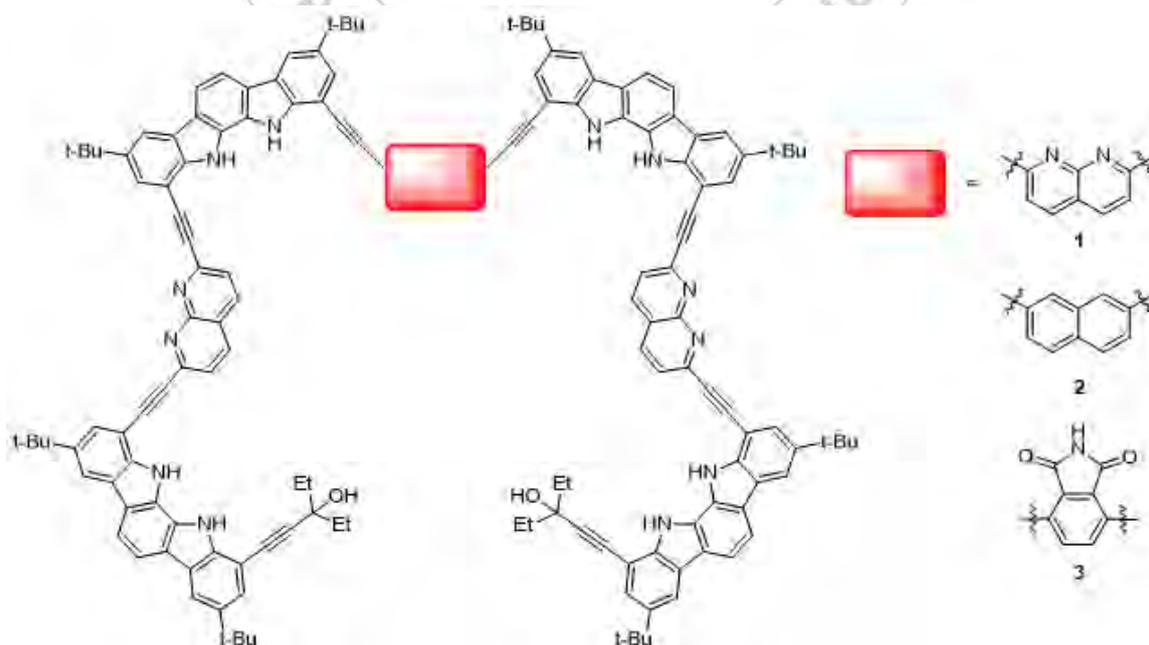
Exhibition Hall 2, THU 11:00~12:30

Functional Indolocarbazole–Naphthyridine Foldamers via the Site-Specific Modification

Woojeong Chae

Chemistry, Yonsei University, Korea

Recently, we demonstrated that indolocarbazole–naphthyridine foldamer (1) adopted a helically folded conformation and bound monosaccharide such as glucose with high affinity and selectivity in solution.¹ However, it was proven to bind glucose only in highly dried solutions because of highly competitive binding of water molecules inside the cavity. Herein, we modify a subunit in the middle of the sequence from naphthyridine to naphthalene (2) or phthalimide (3) that may disrupt and weaken hydrogen bonding with water molecules inside the cavity. As anticipated, these new foldamers adopt helical structures with an internal tubular cavity which can encapsulate appropriate guests. Details including syntheses, structural analyses and binding studies will be discussed in the poster presentation.



Poster Presentation : **ORGN.P-371**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Hole transport layer using azide based photo-crosslinking system for solution-processed organic light-emitting diodes.

Jeong Yong Park, Do-Hoon Hwang*, Jae-Ho Jang

Department of Chemistry, Pusan National University, Korea

We have designed the new system, blending azide photo-cross-linkable moiety to Poly(bis-4-butylphenyl-N,N-bisphenyl)benzidine [Poly-TPD] which is reported as a hole-transporting material, for Solution-Processed Organic Light Emitting Diodes (OLEDs). The useful photo-crosslinking process is demonstrated with UV irradiation (254 nm, 60mw/cm²) at a short exposure time (5s). The photo-crosslinking process occur in benzyl alkyl side-chain insertion reactions, which do not degrade semiconductor properties. It was a good solvent resistances in common organic solvents such as isopropyl alcohol, anisole, toluene, and chlorobenzene. The solution-processed red OLEDs devices fabricated using Poly-TPD with blending azide(1wt%) as a hole-transporting layer (HTL). We fabricated multilayered OLEDs ITO/PEDOT:PSS (30 nm) /Poly-TPD:azide(1wt%) or Poly-TPD (20 nm) /TCTA:TPBi:Ir(piq)₂tmd (5%) /TPBi (40 nm)/ LiF(1 nm)/ Al (100nm) through spin-coating and vacuum deposition. The OLEDs fabricated using HTL with blending azide photo-cross-linkable moiety exhibited significantly improved current efficiency and external quantum efficiency (EQE) compared to HTL without blending azide photo-cross-linkable moiety. It shows maximum luminescence of 3,239 cd/m², maximum luminous efficiency of 13.32 cd/A, power efficiency of 4.11 lm/W, and external quantum efficiency of 9.11%

Poster Presentation : **ORGN.P-372**

Organic Chemistry

Exhibition Hall 2, THU 11:00~12:30

Thermally Cross-Linkable Host materials with styrene for Solution-Processed Organic Light-Emitting Diodes

Jae-Ho Jang, Jeong Yong Park, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

Thermally cross-linkable host materials, DV-TPACZ, DV-TPADBCZ, and TV-TPBI, were designed and synthesized for solution-processed organic light-emitting diodes (OLEDs). The synthesized styrene-functionalized host materials were thermally cross-linked by curing at 150–200 °C without using a polymerization initiator. Excellent solvent resistance was observed for all cured host films. They exhibited low highest occupied molecular orbital energy levels of 5.4–5.7 eV, which indicated a low hole injection barrier from the hole transport layer to the emissive layer. A solution-processed red phosphorescent OLED with 5 wt% (MPHQ)₂Ir(tmd) dopant in the thermally cross-linkable DV-TPACZ host exhibited a current efficiency of 5.3 cd/A, power efficiency of 3.2 lm/W, and external quantum efficiency of 3.6%.

Poster Presentation : **MEDLP-373**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design, Synthesis, and Enzyme Inhibitory Activities against AXL and ACK1 of Novel Aminopyrimidine Derivatives

Juri Suh, Jongseung Kim, Kyung Ho Yoo^{1,*}

Department of Chemistry, Korea University, Korea

¹*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

AXL is a receptor tyrosine kinase involved in the growth, differentiation, survival, and motility of many different cell types. 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 emergence of ACK1 as an oncogenic kinase has uncovered novel mechanisms by which tyrosine kinase signaling promotes cancer progression. 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 kinase inhibitors against AXL and ACK1. Many kinase inhibitors utilize the pyrimidine scaffold as a hinge anchor with various substitutions at 2- and 4-positions. In this work, a novel series of aminopyrimidine derivatives, based on the structural features of TP-0903 and TAE-684 as AXL and ACK1 inhibitors, were designed and synthesized. The *in vitro* enzyme inhibitory activities against AXL and ACK1 for the synthesized compounds were tested.

Poster Presentation : **MEDIP-374**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Identification of novel scaffold inhibitors of mammalian target of rapamycin (mTOR) from high-throughput screening

Sunwoo Lim, Wooyoung Hur^{1,*}

Department of Chemistry, Korea University, Korea

¹*Korea Institute of Science and Technology, Korea*

We performed a high-throughput biochemical screen against mTORC1 using 100,000 small molecule library. Three novel, structurally distinct compounds were identified that inhibited mTORC1 and 2 with IC₅₀'s of less than 10 μ M. Docking study suggested that all three compounds are ATP-competitive and form a hydrogen bond with Val2240 in the hinge region, and some compounds exhibit pi-pi interaction with Trp2239 within the ATP pocket. We prepared several analogues of each hit compound and investigated structure-activity relationship. Our study provides potential starting points for development of new mTOR inhibitors.

Poster Presentation : **MEDIP-375**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

3D Printig feature evaluation of PCL/PEG/Gelatin composited scaffold for cell culture

Sang Hyeob Lee, Il Yoon^{1,*}

Department of Nanoscience, Nano Drug Delivery Lab, Korea

¹PDT Laboratory, Inje University, Korea

The 3D printed scaffold has been used and developed in many areas such as cell experimentation, tissue, bone, skin, cartilage, and implants. Among them, the aim is to develop a scaffold that is used for cell experimentation. Using the synthetic polymers PCL, PEG, and the natural polymer Gelatin, make a simple and reasonable scaffold. It measures and compares material properties, water-solubility, porosity, networkability, and biocompatibility that are important in a scaffold.



Poster Presentation : **MED.P-376**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

1H-indole-3-acetic acid (IAA) derivatives for Butrylcholinesterase Inhibitor

Minji Kim, Haneul Lee, Yujung Kang, Jintaek Oh, Minyeong Choi, Ji Hyun Hwang, Jeong Ho Park^{1,*}

Department of Chemical & Biological Engineering, Hanbat National University, Korea

¹*Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea*

We have been trying to find out new drug candidate compounds for Alzheimer's drugs based on the cholinergic theory. 1H-indole-3-acetic acid (IAA) is one of plant hormones and also shows anti-cancer effect. IAA derivatives were synthesized by the click reaction between propargylated IAA and substituted benzyl azide. *In vitro* cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated by using IAA derivatives. Although the IC₅₀ value of compound **6** is 15.15±0.87μM, it is a little bit less IC₅₀ value than galantamine (IC₅₀ = 9.4±2.5μM against BuChE).

Poster Presentation : **MEDI.P-377**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Identification and Biological Activities of taxifolin in *Wolfiporia extensa*

Sangwoo Kim, Minji Kim, Zhou Xinxin, Bong Ho Lee^{1,*}

Department of Chemical & Biological Engineering, Hanbat National University, Korea

¹*Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea*

In our continuing search for biologically active compounds from oriental medicinal plants, *Wolfiporia extensa* was examined and we have been able to identify taxifolin as an active compound. Here, we report the progress on the purification, identification, and biological activities of the compound. From the 100% methanol extract of *Wolfiporia extensa*, solvent partition were prepared by using *n*-hexane (WEH), chloroform (WEC), butanol (WEB) and water (WEW). Among them, WEB showed strong anti-oxidative and BuChE inhibitory activities. The extracts in WEB of *Wolfiporia extensa* showed 91.3% ABTS radical scavenging activity, and 41.2% BuChE inhibitory activity at 100 ppm. Taxifolin showed 30.1% BuChE inhibitory activity, 94.2% ABTS radical scavenging activity. Bioactive compounds were purified through a series of various chromatographic methods.

Poster Presentation : **MEDLP-378**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design, Synthesis and biological evaluation of novel pyrimidine derivatives as NUA1 kinase inhibitors

JaeHo Kim, Sora Paik¹, So Ha Lee^{2,*}, Jongseung Kim*

Department of Chemistry, Korea University, Korea

¹*Korea Institute of Science and Technology, Korea*

²*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

Abstract Cancer cells grow by the signal transduction pathway like normal cells and there are various protein kinases in the cell that play an important role in the signaling pathway. Until recently, it has been known that among the various kinases, NUA1 kinase has two types of NUA1, NUA2. NUA1 kinase is a serine / threonine protein kinase belonging to the AMP-activating protein kinase (AMPK) family and (AMPK) is a critical regulator of cellular and whole-body energy homeostasis with potential therapeutic targets. ARK5, AMPK – related protein kinase mediating Akt signals, is closely involved in tumor progression, and its stage-associated expression was observed in colorectal cancer. Also, (NUA1) has been reported to promote tumor progression and metastatic capacity via the upregulation of cell proliferation, inhibition of p53-mediated tumor suppression, and increased matrix metalloproteinases (MMPs) in various cancer. More recently, a key finding showing that NUA1 (also known as ARK5) may play a role in regulating tumor proliferation and survival through metabolic alteration in hepatocarcinoma demonstrated that targeting cellular energy homeostasis could be a valuable strategy to eliminate Myc-deregulated tumor cells. Therefore, inhibition of NUA1 can be an effective therapeutic strategy in these diseases. For developing NUA1 inhibitors, From high-throughput screening, we found hit compounds, and synthesized new pyrimidine derivatives based on the hit scaffolds. Among the synthesized compounds, KIST301670 was identified as a potent NUA1 inhibitor. The optimization of novel NUA1 inhibitors to further enhance potency and physicochemical properties is now in progress.

Poster Presentation : **MEDLP-379**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

A novel highly potent and selective 11 β -hydroxysteroid dehydrogenase type 1 inhibitor in a diabetic mouse model

Hanbyeol Park, Dong Oh Han¹, Soon Kil Ahn*

Institute for New Drug Development, Division of Life Sciences, Korea

¹*Biodrug Department, Ahngook Pharm., Korea*

11 β -hydroxysteroid dehydrogenase type 1 (11 β -HSD1) is a cortisol regenerating enzyme that amplifies tissue glucocorticoid levels, especially in the liver and adipose tissue. Knockout mice or a selective inhibitor of 11 β -HSD1 improves metabolic syndrome parameters in preclinical models and human clinical trials. Here, we evaluated the therapeutic potential of INU-101, a potent and selective oral inhibitor of 11 β -HSD1. The *in vitro* activity of 11 β -HSD1 was measured using the homogeneous time-resolved fluorescence (HTRF) assay. Differentiated adipocytes were used to evaluate the cellular 11 β -HSD1 activity. To determine the inhibitory effects on 11 β -HSD1 in tissues, we performed *ex vivo* studies using liver and adipose tissue isolated from C57BL/6J mice and Cynomolgus monkeys. KKAY mice and ZDF rats were administered INU-101 to evaluate whether this compound ameliorated metabolic abnormalities in obese and diabetic animals. INU-101 had highly potent inhibitory activity in mouse, monkey and human 11 β -HSD1, derived from liver microsomes. The oral administration of INU-101 significantly inhibited 11 β -HSD1 activity in the liver and adipose tissue of mice and monkeys. In KKAY mice and ZDF rats, the oral administration of INU-101 enhanced insulin sensitivity and lowered the fasting blood glucose level. Furthermore, INU-101 treatment decreased the body weight and ameliorated an improved lipid profile in the diabetic mouse model. These results suggest that the 11 β -HSD1 inhibitor, INU-101 may serve as a novel drug candidate for the treatment of type 2 diabetes and metabolic syndrome.

Poster Presentation : **MED.P-380**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Efficient and rapid synthesis of N-substituted isoquinolin-1(2H)-one under mild conditions: Facile access to doryamine derivatives

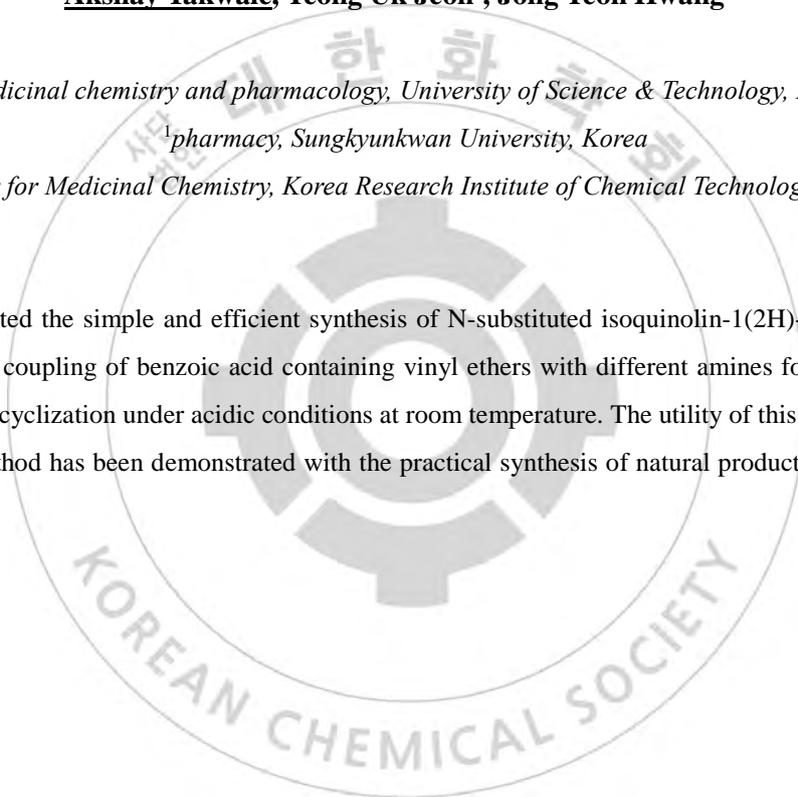
Akshay Takwale, Yeong Uk Jeon¹, Jong Yeon Hwang^{2,*}

Medicinal chemistry and pharmacology, University of Science & Technology, India

¹*pharmacy, Sungkyunkwan University, Korea*

²*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

We have depicted the simple and efficient synthesis of N-substituted isoquinolin-1(2H)-one derivatives. Initiating from coupling of benzoic acid containing vinyl ethers with different amines followed by rapid intramolecular cyclization under acidic conditions at room temperature. The utility of this simple and mild cyclization method has been demonstrated with the practical synthesis of natural product, doryamine and its analogues



Poster Presentation : **MEDLP-381**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

EGFR exon 20 insertion mutations to NSCLC

Jiwon Kim, Chong Hak Chae¹, Kwangho Lee^{1,*}

medicinal chemistry and pharmacology, Korea Research Institute of Chemical Technology, Korea

¹*Korea Research Institute of Chemical Technology, Korea*

Non-small cell lung cancer (NSCLC) is one of the leading causes of cancer-related death globally. Exon 20 insertion mutations are the third EGFR mutations in NSCLC. It reportedly relates from 1.5% to 10 % of all EGFR mutations. Most of the mutations occur at the short loop connecting the α C-helix and β 4 strand after Methionine 766. NSCLC patients caused by Exon 20 insertion mutations have received little benefits with the approved EGFR first-generation TKIs. So, there is unmet medical needs for exon 20 insertion mutation inhibitors for NSCLC patients. So far the detail mechanism for this mutation to EGFR overexpression is not fully understood. Cell-based mutation screening reveals the exact location, length, and sequence of the insert mutation matter. Also, it was found that it is important for ligand-independent EGFR activation and down signaling pathway. As a result, N771 P772 INSN, D770N771 INSG, D770>GY were identified as the major factors activating EGFR.

Poster Presentation : **MEDIP-382**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Induced target degradation of BET by target degraders(TDs)

**AhRa Go, Jae du Ha¹, Jong Yeon Hwang*, Yeong Uk Jeon², Pilho Kim, Sung Yun Cho¹,
Chunghoon Shin³, Hyung Soo Kim⁴, WooRi Lee⁵**

Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea

¹*WCI, Korea Research Institute of Chemical Technology, Korea*

²*pharmacy, Sungkyunkwan University, Korea*

³*organic chemistry, Sogang University, Korea*

⁴*organic chemistry, Korea University, Korea*

⁵*Drug discovery, Chungnam National University, Korea*

Immunomodulatory drugs (IMiDs) exert anti-myeloma activity by binding to the protein cereblon (CRBN) and subsequently degrading IKZF1/3. Recently, their ability to recruit E3 ubiquitin ligase has been used in the proteolysis targeting chimera (PROTAC) technology. Of these, BRD4 is the most commonly-targeted protein in PROTAC technology. Herein, we synthesize the TD-428, which comprises TD-106 linked to a BET inhibitor, JQ1 efficiently induce BET protein degradation in the prostate cancer cell line 22Rv1. Consequently, cell proliferation is inhibited due to suppressed C-MYC transcription.

Poster Presentation : **MEDIP-383**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Discovery and Development of Allosteric Inhibitors of Kidney Type Glutaminase with high PK Properties and good Solubility.

Krishna babu Duggirala, Seonghyeon Sim¹, Heeyeon Kang², Yueun Hwang³, Ge Hyeong Lee⁴, Kwangho Lee^{5,*}

University of Science & Technology, India

¹*Chemistry, Sogang University, Korea*

²*Ewha Womans University, Korea*

³*Chemistry, Kwangwoon University, Korea*

⁴*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

⁵*Korea Research Institute of Chemical Technology, Korea*

Glutamine is the most abundant amino acid in the blood. Glutaminase catalyzes the hydrolysis of glutamine into glutamate and ammonia in mitochondria through glutaminolysis. Warburg effect explains glutaminolysis is the main energy source for the growth and viability of malignant tumors. Two isoforms of glutaminase exists in mammalian cells, i.e. kidney type glutaminase (GLS) and liver-type glutaminase (GLS2). GLS was found to be overexpressed in many glutamine dependent cancer cells. Therefore, GLS has become a key target for small molecule therapeutic intervention. Numerous competitive inhibitors (DON) and allosteric inhibitors (BEPTS and CB- 839) were developed. However to date, only CB-839 have entered clinical trials for the treatment of advanced solid tumors and hematological malignancies. Although, several potent inhibitors have been developed, the drug-like properties need to be optimized. Combination of inhibitors with efficient GLS inhibitors could be a potential strategy for patients harboring glutaminase dependent tumors.

Poster Presentation : **MEDLP-384**

Medicinal Chemistry

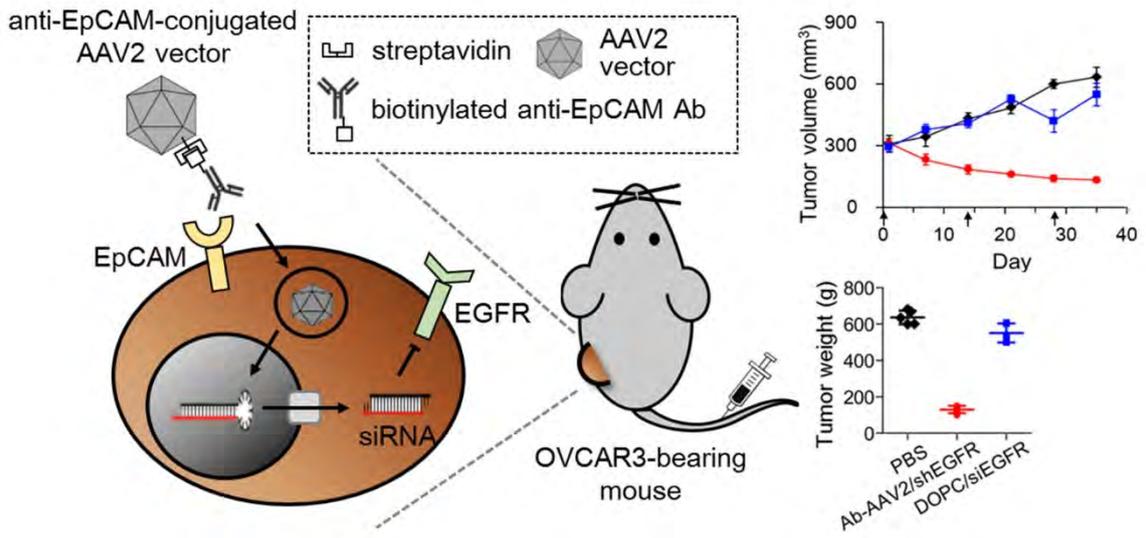
Exhibition Hall 2, THU 11:00~12:30

Retargeting and antitumor effects of adeno-associated virus on OVCAR3 ovarian cancer in vivo

Hyung Jun Ahn

Center for Theragnosis, Korea Institute of Science and Technology, Korea

Adeno-associated virus (AAV) is a promising vector for systemic delivery of siRNA due to its long-term expression ability without immunogenicity and pathogenicity. However, its broad host tropism and lack of tissue specificity has limited clinical applications such as cancer therapy. Therefore, redirecting the natural tropism of AAV vectors to unique cell surface antigens is an important requirement for in vivo RNAi-based cancer therapy. To exploit the overexpression property of epithelial cell adhesion molecule (EpCAM) in specific cancer types, we here created anti-EpCAM antibody-conjugated AAV serotype 2 (AAV2) vectors through a streptavidin-biotin bridge. Upon intravenous injection, anti-EpCAM-conjugated AAV2 vectors showed prominent tumor-specific accumulation in EpCAM-positive tumor-bearing mice without undesirable sequestration in liver. In addition, when loaded with transgenes to express shRNA against epidermal growth factor receptor (EGFR), systemically injected anti-EpCAM-conjugated AAV2/shEGFR vectors induced significant downregulation of EGFR expression in tumors, and eventually suppressed tumor growth even at the long dosing interval of two weeks. This in vivo antitumor effect represents the increased infection efficacy of tropism-modified AAV2 vectors and prolonged expression of EGFR shRNA in tumor tissues. Thus, this study suggests the great potential of anti-EpCAM-conjugated AAV2/shEGFR vectors as RNAi-based cancer therapeutics.



Poster Presentation : **MEDIP-385**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of NIR imaging probes for diagnosis of Alzheimer's disease

Yihoon Kim, Sun-Joon Min*

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

Alzheimer's disease (AD) is a progressive neurodegenerative disease, which causes cognitive deficits that worsen over years. It may be the most costly diseases for society, which will probably increase with the ageing of society, becoming an important social problem. Clinical trial evidence shows that early recognition of cognitive impairment and clinical management at mild stages of AD delays the subsequent need for nursing home care. Consequently, it reduces the risk of misdiagnosis and inappropriate management. A β plaques and tau aggregates, characteristics of AD progression, have been used as biomarkers for diagnosis and monitoring of Alzheimer's disease. Fluorescence imaging is an ideal method to detect the A β plaques and tau aggregates due to its low cost, real time, and highly sensitive detection. Various chemical probes based on fluorescence dyes have been reported, but their low specificity to A β or tau proteins was not suitable for clinical application. Therefore, the development of new near-infrared fluorescence probes targeting these protein aggregates selectively are needed for diagnosis of Alzheimer's disease, in particular, early disease progression. In this report, we describe the synthesis of novel near-infrared fluorescence probes that selectively bind to A β and tau proteins. Based on our preliminary studies, we designed a series of compounds consisting of amino pyridine and dicyano indanes, which were synthesized by palladium-catalyzed coupling reactions and Knoevenagel condensations. Evaluation of the physicochemical properties of these probes and their biological efficacies against A β and tau proteins confirmed the possibility of their use as NIR fluorescent probes for diagnosis of Alzheimer's diseases.

Poster Presentation : **MEDLP-386**

Medicinal Chemistry

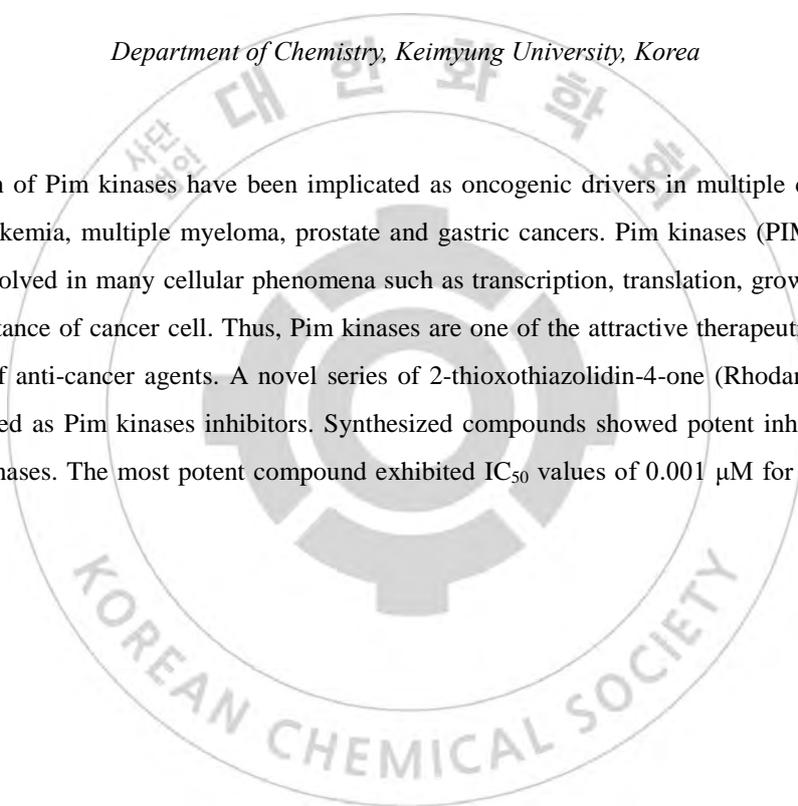
Exhibition Hall 2, THU 11:00~12:30

2-Thioxothiazolidin-4-one derivatives as Pim kinase inhibitors

Yanghwan Yun, Victor Sukbong Hong, Jinho Lee*

Department of Chemistry, Keimyung University, Korea

Overexpression of Pim kinases have been implicated as oncogenic drivers in multiple cancer including lymphoma, leukemia, multiple myeloma, prostate and gastric cancers. Pim kinases (PIM-1, PIM-2, and PIM-3) are involved in many cellular phenomena such as transcription, translation, growth, survival and apoptosis resistance of cancer cell. Thus, Pim kinases are one of the attractive therapeutic targets for the development of anti-cancer agents. A novel series of 2-thioxothiazolidin-4-one (Rhodanine) derivatives were synthesized as Pim kinases inhibitors. Synthesized compounds showed potent inhibitory activities against Pim kinases. The most potent compound exhibited IC₅₀ values of 0.001 μ M for both PIM-1 and PIM-3.



Poster Presentation : **MEDLP-387**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Microwave-Assisted Facile Synthesis of 2,5-Piperazinedione Skeleton

Si Yeon Han, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Many researchers have conducted study about biological activities of 2,5-piperazinedione due to its structural similarities with peptides. The potential of the 2,5-piperazinedione scaffold to serve as a privileged structure for the generation of drug-like libraries in drug discovery program has been plentifully demonstrated in various therapeutic areas such as anti-inflammatory, antimicrobial, anticonvulsant, and antihypertensive. So, we were highly interested in the 2,5-piperazinedione moiety. In this work, we described synthesis of 2,5-piperazinedione derivatives in solution phase. This synthetic methodology involves the preparation of 2,5-piperazinedione skeleton through cyclization of methyl 2-(2-(amino)acetamido)acetate derived from a reaction between *N*- α -chloroacetyl amino acid methyl ester and various amines. Even though several synthesis routes of 2,5-piperazinedione skeleton derived from a reaction between *N*- α -chloroacetyl amino acid methyl ester and amines in 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. It is well known that Microwave reaction in chemical synthesis can decrease reaction time dramatically and generate the desired compounds in high yields and purities at low cost compared to conventional thermal heating. So, we obtained 2,5-piperazinedione in a effective way successfully. Here in, we report an efficient method for the synthesis of 2,5-piperazinedione derivatives based on the combinatorial chemistry techniques.

Poster Presentation : **MEDLP-388**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Solid-Phase Synthesis of 2-Amino-5-Carboxamide Thiazole derivatives via Dehydrative Cyclization of Thiourea Intermediate Resin

Ye Ji Kim, Young Dae Gong*

Department of Chemistry, 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 synthesized using α -bromoketone in the presence of the DMF to afford 2-amino-5-carboxylate thiazole resin. Resulting resin is coupled with various amines. Finally, the 2-amino-5-carboxamide thiazole resin was cleaved from the polymer support using TFA and DCM cocktail. The physicochemical properties of proposed 2-amino-5-carboxamide thiazole derivatives were calculated which shows reasonable oral bioavailability drug properties as determined by the Lipinski's Rule.

Poster Presentation : **MEDIP-389**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Solid-Phase Parallel Synthesis of 1,3-thiazole Derivatives Based on Peptidomimetics

Min jeong Cha, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Synthesis of peptidomimetics has known to be effective for better understanding of protein aggregation which causes neurodegenerative diseases such as Alzheimer's disease. In this work, solid-phase synthesis of 1,3-thiazole derivatives based on peptidomimetics is described. The synthetic strategy starts from constructing 1,3-thiazole core skeleton resin by cyclization of resin-bound cyanocarboimidodithioic acid with ethyl bromoacetate. The resulting core skeleton has amino group and carboxylic acid group which subsequently undergoes functionalization with various amino acids by amide coupling. The desired product has core skeleton of 1,3-thiazole with two sets of three successive amino acids. Trifluoroacetic acid (TFA) in dichloromethane (DCM) is used for cleaving the resin.

Poster Presentation : **MEDLP-390**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design and Solid-Phase Parallel Synthesis of 2,4,5-Trisubstituted Thiazole Derivatives via Cyclization Reaction with a Carbamimidothioate Linker

Hyejin Kwon, Hyungha Park, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Preparation of 2,4,5-trisubstituted thiazole derivatives via a new solid-phase synthetic route has been conducted in this study. The synthetic route begins with synthesis of a core skeleton 2,4-diamino(thiazole-5-yl)substituted-phenylmethanone resin, obtained through a cyclization reaction with a carbamimidothioate linker. The core skeleton was substituted with diverse building blocks such as amines, alkyl halides, and acid chlorides. The products were cleaved from the solid support via TFA/CH₂Cl cleavage cocktail. Overall, the strategy permits the incorporation of three points of diversity into the thiazole ring system with good overall yields.¹ Finally, 2,4,5-trisubstituted thiazole derivatives library showed oral bioavailability through calculation of the physicochemical properties.

Poster Presentation : **MEDI.P-391**

Medicinal Chemistry

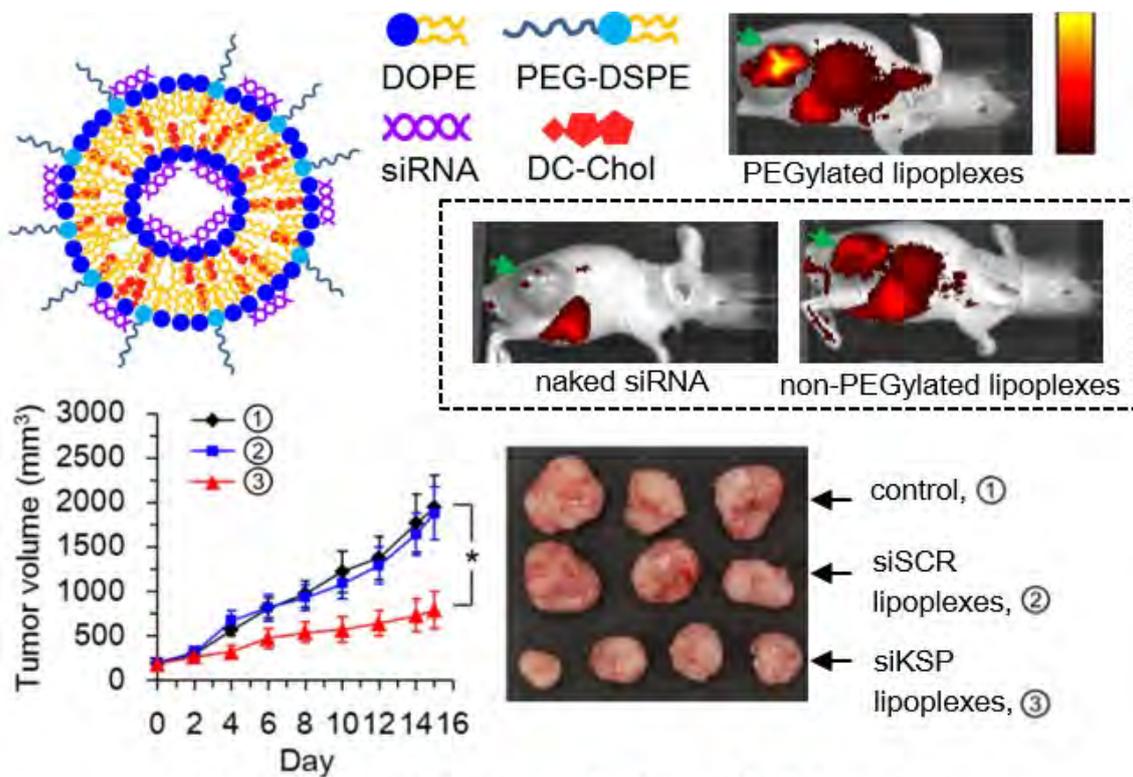
Exhibition Hall 2, THU 11:00~12:30

PEGylated DC-Chol/DOPE cationic liposomes containing KSP siRNA as a systemic siRNA delivery carrier for ovarian cancer therapy

Hyung Jun Ahn

Center for Theragnosis, Korea Institute of Science and Technology, Korea

Although siRNA-mediated downregulation technology has been highly successful in suppressing the expression of any disease-related gene, systemic delivery of siRNA for the clinical applications remains challenging, especially in the use of cancer therapy. DC-Chol/DOPE cationic liposomes as one of the most attractive vehicles for gene delivery have been widely exploited for transfection of siRNA into cells, but complexity of systemic delivery has allowed only their direct injection into local targets due to the formation of aggregations with negatively-charged blood components. Herein, we demonstrate the effects of PEGylation on DC-Chol/DOPE cationic liposomes for systemic siRNA delivery in cancer therapy. In contrast to non-PEGylated DC-Chol/DOPE-siRNA lipoplexes, PEGylated DC-Chol/DOPE-siRNA lipoplexes reduce the excretion by kidneys and scavenging in liver, prolonging the circulation time in vivo, and ultimately increase their preferential tumor accumulation. Therefore, systemic injection of PEGylated DC-Chol/DOPE liposomes loaded with siRNA against kinesin spindle protein (KSP) gene exhibited a high level of target gene silencing at tumor sites and substantial suppression of tumor growth. Furthermore, systemically administered PEGylated lipoplexes did not lead to any activation of innate immune responses in the immunocompetent mice. These results suggest the potential of PEGylated DC-Chol/DOPE liposomes as a systemic delivery carrier for siRNA-mediated cancer therapy.



PEGylated DC-Chol/DOPE-siRNA lipoplex



Poster Presentation : **MEDIP-392**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Tau-Targeted Drug Discovery for the Treatment of Alzheimer's Disease

Haeun Lee, Ae Nim Pae^{1,*}, Sang Min Lim^{1,*}

University of Science and Technology, Korea

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 : **MEDLP-393**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Potent β -Arrestin-biased S1P₁ Agonist for Treatment of Multiple Sclerosis

Jee yun Ahn, WooSeung Son¹, Kyu-Sung Jeong¹, Jong-Hyun Park², Ki Duk Park³, Sang Min Lim⁴, Ae Nim Pae^{4,*}

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Multiple sclerosis (MS) is a T-cell mediated autoimmune disease of the CNS. Fingolimod is the first FDA-approved drug for relapsing MS. In Human clinical trials, it is associated with side effects such as hypertension by non-selective S1P_{1,3,4,5} receptors agonism.¹ Our reason for developing potent and selective S1P₁ receptor agonist is to be lower the circulating lymphocytes more efficiently by internalization of S1P₁ on lymphocyte.² We designed and synthesized S1P₁ receptor agonists with selectivity against S1P₃ receptor via in silico docking study on S1P₁ receptor crystal structure. Among synthesized compounds, S38 showed remarkable in vitro activities (Ca²⁺ signaling assay, EC₅₀= 35 nM, β -arrestin assay, EC₅₀= 0.2 nM and internalization assay, EC₅₀= 2.8 nM) with sparing activity against S1P₃ receptor. Furthermore, the compound S21 exhibited β -arrestin biased signaling as S1P₁ agonist (Ca²⁺ signaling assay, EC₅₀= 1.86 μ M, β -arrestin assay, EC₅₀= 8.9 nM and internalization assay, EC₅₀=32 nM). The selected compounds, S21, S38 and S40, are being performed peripheral lymphocyte counting assays. The optimization is now in progress on enhancing potency and pharmacokinetic properties to synthesize novel S1P₁ agonist.

Poster Presentation : **MEDIP-394**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Location of peptide assembly determines the death mechanism

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

Peptide sequence can be designed to form supramolecular structure such as fiber, tube and vesicle structure via self-assembly. When each peptide monomer and their aggregated state reach to equilibrium state, self-assembly process was occurred. Therefore, the concentration is the critical controllable factor to induce assembly. Self-assembly appears when molecules achieve critical aggregation concentration, CAC. In living cells, designed molecules form the self-assembly structure over the CAC inside targeted organelle then it induce the severe damage to cell. Our group previously made the amphiphilic peptide, Mito-FF. It was designed to accumulate in mitochondria. The sequence of Mito-FF is 'Pyrenebutyric acid-FFK-TPP'. Diphenylalanine(FF) form the β -sheet domain, triphenylphosphonium(TPP) is the mitochondria targeting moiety it was conjugated on lysine. We chose the target organelle as mitochondria because mitochondria has important role in metabolism, regulator of cell death. And pyrene as a fluorescence group to observe uptake on mitochondria. To understand how small molecule conjugated to N-terminal on peptide sequence can affects to cell death, 5 small molecule was used for synthesize Mito-FF based peptides. Octanoic acid, palmitic acid, pefluorooctanoic acid, nitrobenzodiazole(NBD), naphthalene tetracarboxylic dianhydride was used. Especially, Palmitic acid showed different tendency compare to Mito-FF. Mito-FF is known as induce apoptosis. In contrast, palmitic acid(C16) conjugated FFK-TPP molecule induced necrosis. To observe this different death mechanism, we synthesized C16-FFK(NBD)K(TPP) and Pyrenebutyric acid-FFK(NBD)K(TPP). NBD dye was selected for confocal microscopy. Two product was incubated both cancer cell(HeLa) and normal cell(NIH-3T3).

Poster Presentation : **MEDIP-395**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

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

Youjung Sim, Myoung Soo Lah*, Ja-Hyoung Ryu*

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

Photodynamic Therapy (PDT) is a form of a phototherapy inducing cell death using light, oxygen and Photosensitizer(PS) which is generating ROS. These ROS interact with cellular components including lipids, amino acid and nucleic acids, and lead to the cell dysfunction. However, as a tumor grows, it rapidly outgrows its blood supply, leaving portions of the tumor where the oxygen concentration is significantly lower than in healthy tissues. For this reason, even effective photosensitizers cannot be working efficiently as much as expected. Therefore, if we overcome this hypoxia environment of tumor, photodynamic therapy can be more effective way forward. In our research, we conjugate the enzyme catalase(CAT) to surface of biocompatible nanocarrier MOF808. Catalase catalyzes the decomposition of hydrogen peroxide (H_2O_2) to water(H_2O) and oxygen(O_2). The generated oxygen can relieve the Hypoxia condition in tumor. Enriched oxygen further increases the PDT effect, enabling effective ROS generation. Also, immobilized enzyme is more stable than the free form of the enzyme enhancing the recyclability of enzymes and minimizing enzyme contamination.

Poster Presentation : **MEDLP-396**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and Evaluation of Novel Functionalized Amino Acid Derivatives for Treatment of Cryptococcal Meningitis

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Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

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 **KDS5098** through MIC testing for representative fungal pathogens. (MIC: *C. neoformans* = 4 g/mL, *C. albicans* = 16 g/mL). Herein, we optimized lead compound for both the antifungal efficacy and drug-like properties. Among the optimized compounds, **KDS6002** showed the similar antifungal efficacies (MIC: *C. neoformans* = 2 g/mL, *C. albicans* = 6 g/mL). Furthermore, **KDS6002** improved ADME/Tox profiles (microsomal stability (human): 96%, (mouse) 100% remaining after 30 min; CYP inhibition (1A2, 2C9, 2C19, 2D6): IC₅₀ > 10 μM, (3A4; 72% inhibition at 10 μM); Pharmacokinetics: *F* = 95%).

Poster Presentation : **MEDIP-397**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development and Optimization of Halogenated Vinyl Sulfones as Nrf2 Activators for the Treatment of Parkinson's Disease

Jong Seok Yoo, Ki Duk Park*

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

Parkinson's disease (PD) is a common neurodegenerative disorder which is characterized by abnormalities in motor control and muscle rigidity. Recent studies suggest that oxidative stress causes the striatal dopamine (DA) deficiency by neuronal loss in the substantia nigra (SN). The Nrf2 signaling is the main pathway responsible for cellular defense system against oxidative stress. Nrf2 is a transcription factor that regulates environmental stress response by inducing expression of various antioxidant enzyme genes. In previous work, we have synthesized novel vinyl sulfone derivatives as Nrf2 activator. The lead compound **KDS4048** was confirmed to activate Nrf2 and to induce expression of the Nrf2 dependent antioxidant enzymes such as NQO1, GCLC, GLCM, and HO-1 at both mRNA and protein levels in dopaminergic neuronal cells. In this work, we have optimized the lead compound **KDS4048** ($EC_{50}=530$ nM) to improve drug-like properties and increase potency of Nrf2 activation. Compounds were synthesized by introducing halogen groups and pyridine ring into the vinyl sulfones. Among the synthesized compounds, **KDS7001** and **KDS7011** exhibited potent effect on Nrf2 activation (**KDS7001** $EC_{50}=217$ nM, **KDS7011** $EC_{50}=213$ nM) in cell-based assay. We will further evaluate whether two compounds induce the expression of antioxidant response genes NQO1, GCLC, GLCM, and HO-1 at both mRNA and protein levels and attenuate the PD-like motor dysfunctions in the MPTP-induced mice model of PD.

Poster Presentation : **MEDIP-398**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

Hye Yeon Lee, Haeun Lee¹, WooSeung Son², Ae Nim Pae³, Hak Joong Kim^{*}, Sang Min Lim^{3,*}

Department of Chemistry, Korea University, Korea

¹*Biochemistry, Korea University of Science and Technology, Korea*

²*Department of Chemistry, Yonsei University, Korea*

³*Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is one of the most common neurodegenerative diseases and becomes a serious problem in an aging society. Tau is a microtubule-associated protein and is believed to play an important role in AD pathology. Tau protein binds to microtubules and helps stabilize neuronal microtubules. However, hyperphosphorylation of tau causes dissociation from microtubules, and detached tau proteins tend to self-assemble eventually forming paired helical filaments (PHFs) and neurofibrillary tangles (NFTs). Finally, these PHFs and NFTs can induce neurodegeneration leading to diseases like AD. Despite the importance of treatment of AD, there are drugs that only alleviate some of the symptoms of AD. Therefore, we pay attention to the pathological characters of tau protein, and intend to develop tau aggregation inhibitors to find disease-modifying drug candidates for AD therapy. To discover new lead compounds that can inhibit tau aggregation, we performed a high-throughput screening based on a Bi-FC assay with in-house libraries. Thereafter, by modifying hit compounds, we found compounds that are more potent and less toxic than Methylene blue: a well-known *in vitro* tau aggregation inhibitor. Currently, we have synthesized a variety of derivatives through a structure-activity relationship study to find compounds that are more potent than the hit compounds. We are also trying to find potent compounds possessing novel scaffolds by introducing bioisosteres. We will continue our efforts to optimize potency as well as physicochemical properties to develop non-clinical candidates for AD.

Poster Presentation : **MEDIP-399**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Discovery of Potent, Selective, and Orally Bioavailable Estrogen-Related Receptor- γ Inverse Agonists

Jina Kim, Jungwook Chin*, Sung Jin Cho*

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

ERR γ is abundantly expressed in various tissues associated with the CNS, circadian clock, and basal metabolic function; thus, it not only regulates ion homeostasis in related tissues but also controls metabolic processes such as mitochondrial biogenesis and hepatic gluconeogenesis. We synthesized potent, selective and orally bioavailable ERR γ inverse agonists and evaluated the in vitro pharmacology as well as the absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of chemical entities that not only were shown to be highly selective inverse agonists for ERR γ but also exhibited enhanced pharmacokinetic profile compared with GSK5182. We observed a significant increase of fully glycosylated NIS protein, key protein for radioiodine therapy in anaplastic thyroid cancer (ATC), in DN201000-treated CAL62 cells, which indicated that these compounds could be promising enhancers for restoring NIS protein function in ATC cells. Thus, DN201000 possess advantageous druglike properties and can be used to potentially treat various ERR γ -related disorders.

Poster Presentation : **MEDIP-400**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of Novel biased agonists against S1P1 receptor for Treatment of Multiple Sclerosis

Sun Jun Park, Ki Duk Park*

Convergence Research Center for DTC, Korea Institute of Science and Technology, Korea

The sphingosine-1-phosphate (S1P) receptors are the initial lipid G protein-coupled receptors (GPCRs) that are divided into five subtypes; S1P1, S1P2, S1P3, S1P4, and S1P5. In particular, targeting S1P1 with the endogenous ligand, S1P, has shown substantial efficacy in treatment of multiple sclerosis (MS) since it promotes egress of lymphocytes from lymph nodes. The S1P receptor agonist has been shown to induce receptor down-regulation from the cell surface, suggesting that it acts as a functional antagonist of S1P1 to block lymphocyte egress by internalization of the receptor. In this study, we synthesized a series of chemical derivatives to deduce a potent lead compound and evaluated their biological activities and selectivity using a set of complementary assays such as Ca⁺⁺ flux, cAMP assay, β -arrestin recruitment, and S1P1 receptor internalization. Among the synthesized compounds, KDS1059 exhibited potent activities on β -arrestin recruitment and S1P1 receptor internalization with an EC₅₀ of 180 nM and 10 nM, respectively, whereas it was slightly active (EC₅₀=1.72 μ M) on Ca⁺⁺ assay indicating that KDS1059 is a biased agonist. As a continuation of these efforts, we replaced the core part of KDS1059 and we synthesized the KDS8000 series compounds. Among them, KDS8007 has a marvelous efficacy. KDS8007 exhibited potent activities on β -arrestin recruitment and Ca⁺⁺ assay with an EC₅₀ of 0.37 nM and 96.5 nM, respectively, KDS8007 has approximately 30-fold β -arrestin recruitment than KDS1059. Additionally we are still working on this study. References Birker-Robaczewska, M. etc., al. Mol Pharmacol. 2018, 93, 109-118. Cohen, J. etc., al. Ann Neurol. 2011, 69, 759-777. Marsolais, D. etc., al. Nat Rev. 2009, 8, 297-307.

Poster Presentation : **MEDLP-401**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Novel tau aggregation inhibitors for treatment of Alzheimer's Disease

WooSeung Son, Sang Min Lim¹, Kyu-Sung Jeong, Ae Nim Pae^{1,*}

Department of Chemistry, Yonsei University, Korea

¹Convergence Research Center For Diagnosis, Treatment and Care System of Dementia, Korea Institute of Science and Technology, Korea

Alzheimer's disease(AD) is a chronic neurodegenerative disease that is the most common form of dementia. It is still unknown what AD causes, but AD features two histopathological hallmarks : amyloid plaques(AP) made of amyloid- β and neurofibrillary tangles(NFTs) arising from the hyperphosphorylated tau aggregation in pathology. It is known AP and NFT are neurotoxic that may lead to impairment of brain. In clinical trials, diverse compounds, such as amyloid aggregation inhibitors, β -secretase inhibitors and so on, have been failed to cure AD patients. Therefore, our rationale of tau aggregation inhibitors reduce the generation of NFT that may relate to causes of AD. We identified lead compound (DTC0100) which inhibits tau aggregation by high contents screening in Tau Bi-FC cell-based assays. Then, a variety of derivatives were synthesized through a structure-activity relationship study and the optimization of novel tau aggregation inhibitors to improve potency, physicochemical properties and in vivo efficacy. Among synthesized compounds, DTC0521 showed excellent inhibitory activity of tau aggregation ($IC_{50} = 0.06 \mu M$) in Tau Bi-FC assays and was also lower tau aggregation ($IC_{50} = 0.58 \mu M$) in ThS assays. DTC0521 showed the recovery of cognitive impairments (Tau-P301L-BiFC transgenic mice) in behavior test and decreases tau aggregation as well as phosphorylated tau. It also exhibited good pharmacokinetic profile and ADME/Tox, thus, the validation of DTC0521 as preclinical candidate and further optimization are in progress.

Poster Presentation : **MEDI.P-402**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Novel Chalcone Derivative Suppress Inflammation via Nrf2 Activation and Attenuates the Learning and Memory Impairment in Scopolamine-Induced Mouse Model

Boko Jang, Ki Duk Park*

Convergence Research Center for DTC, Korea Institute of Science and Technology, Korea

Alzheimer's disease (AD) is a common neurodegenerative disease characterized by progressive degeneration and neuronal cell death, resulting in neural network dysfunction. As the underlying mechanisms, oxidative damage and neuroinflammation have been reported to contribute to the onset and deterioration of AD. Nrf2-ARE signaling pathway is a pivotal cellular defense mechanism against oxidative stress. Nrf2, a transcription factor, regulates the cellular redox balance and is also primarily involved in anti-inflammatory response. Here, we have synthesized novel chalcone derivatives and found a highly potent Nrf2 activator, compound **9a**. Compound **9a** induced expression of Nrf2-dependent antioxidant enzymes, increased SOD activity, and inhibited reactive oxygen species production. It also suppressed the production of nitric oxide and down-regulated inflammatory mediators confirming its anti-inflammatory effect. In addition, compound **9a** effectively recovered the learning and memory impairment in scopolamine-induced amnesia model.

Poster Presentation : **MEDLP-403**

Medicinal Chemistry

Exhibition Hall 2, 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, Haeun Lee, Hyeon Jeong Kim, Boko Jang, Jaeick Lee¹, Sang Min Lim, Ae Nim Pae*, Ki Duk Park*

Convergence Research Center for DTC, Korea Institute of Science and Technology, Korea

¹Doping Control Center, 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. Oxidative stress has been 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-404**

Medicinal Chemistry

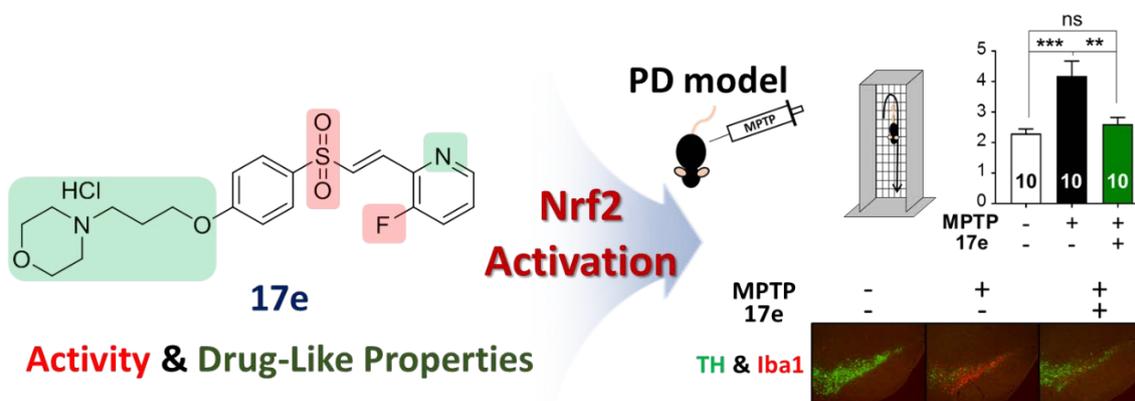
Exhibition Hall 2, THU 11:00~12:30

Design, Synthesis and Optimization of Novel Class of Nrf2 Activator as a Neuroprotective Agent for Treatment of Parkinson's disease

Ji Won Choi, Siwon Kim, Jong-Hyun Park, Hyeon Jeong Kim, Hyeon Ji Kim, Boko Jang, Sun Jun Park, Jong Seok Yoo, Areum Song, Ki Duk Park*

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

We previously developed a novel series of vinyl sulfones as nuclear factor erythroid 2-related factor 2 (Nrf2) activators with therapeutic potential for Parkinson's disease (PD). However, the previously developed lead compound (**1**) exhibited undesirable drug-like properties. Here, we optimized vinyl sulfones by introducing nitrogen heterocycles to improve drug-like properties. Among the synthesized compounds, **17e** was the most promising drug candidate with good drug-like properties. Compound **17e** showed superior effects on Nrf2 activation in cell-based assays compared to compound **1** (**17e**: EC₅₀ = 346 nM; **1**: EC₅₀ = 530 nM). Compound **17e** was further confirmed to induce expression of Nrf2-dependent antioxidant enzymes at both mRNA and protein levels. In a 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP)-induced mouse model of PD, **17e** significantly attenuated loss of tyrosine hydroxylase-immunopositive dopaminergic neurons, suppressed microglial activation, and alleviated PD-associated motor dysfunction. Thus, **17e** is a novel Nrf2 activator with excellent drug-like properties and represents a potential therapeutic candidate for PD.



Poster Presentation : **MEDLP-405**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Niclosamide derivatives inhibit CIP2A and reactivate tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells.

Seokjun Jo, Seung Kyu Kang¹, Moon Gyu Baek¹, Kwan-Young Jung^{2,*}

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Protein phosphatase 2A (PP2A) is a critical tumor suppressor complex responsible for the inactivation of various oncogenes. Recently, PP2A reactivation has emerged as an anticancer strategy. Cancerous inhibitor of protein phosphatase 2A (CIP2A), an endogenous inhibitor of PP2A, is upregulated in many cancer cells, including non-small cell lung cancer (NSCLC) cells. We demonstrated that the antihelminthic drug niclosamide inhibited the expression of CIP2A and reactivated the tumor suppressor PP2A in NSCLC cells. We performed a drug-repurposing screen and identified niclosamide as a CIP2A suppressor in NSCLC cells. Niclosamide inhibited cell proliferation, colony formation, and tumor sphere formation, and induced mitochondrial dysfunction through increased mitochondrial ROS production in NSCLC cells; however, these effects were rescued by CIP2A overexpression, which indicated that the antitumor activity of niclosamide was dependent on CIP2A. We found that niclosamide increased PP2A activity through CIP2A inhibition, which reduced the phosphorylation of several oncogenic proteins. Moreover, we found that a niclosamide analog inhibited CIP2A expression and increased PP2A activity in several types of NSCLC cells. Finally, we showed that other well-known PP2A activators, including forskolin and FTY720, did not inhibit CIP2A and that their activities were not dependent on CIP2A. Collectively, our data suggested that niclosamide effectively suppressed CIP2A expression and subsequently activated PP2A in NSCLC cells. This provided strong evidence for the potential use of niclosamide as a PP2A-activating drug in the clinical treatment of NSCLC.

Poster Presentation : **MEDIP-406**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Design, synthesis and biological evaluation of phenoxazine derivatives as clathrin inhibitors

Eunyeong Rim, Seung Kyu Kang¹, Chijung Kim¹, Navin Pandit, Kwan-Young Jung^{1,*}

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

¹*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Clathrin regulates various physiological processes, including internalization of growth factors and receptors, synaptic transmission, and entry of pathogens. Clathrin functions as a central organizing platform for coated pit assembly and dissociation within the endocytic network through its terminal domain. To inhibit clathrin, a series of phenoxazine compounds were synthesized and evaluated for their clathrin inhibitory effect by measuring transferrin uptake and change of puncta. Among the phenoxazine derivatives, 3-(10H-phenoxazin-10-yl)-N,N-bis(2-((tetrahydro-2H-pyran-2-yl)oxy)ethyl)propan-1-amine (3t) was identified as the best clathrin inhibitor with $IC_{50} = 6.8 \mu M$.

Poster Presentation : **MEDIP-407**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Newly developed reversible MAO-B inhibitor circumvents the shortcomings of irreversible inhibitors in Alzheimer's disease

Jong-Hyun Park, Ji Won Choi, Boko Jang, Hyeon Jeong Kim, Siwon Kim, Ki Duk Park*

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

Monoamine oxidase-B (MAO-B) has recently emerged as a potential therapeutic target for Alzheimer's disease (AD) due to its association with aberrant gamma aminobutyric acid (GABA) production in reactive astrocytes. Although short-term treatment with irreversible MAO-B inhibitors, such as selegiline, improves cognitive deficits in AD patients, long-term treatments have shown disappointing results. Here, we show that prolonged treatment with selegiline fails to reduce aberrant astrocytic GABA levels and rescue memory impairment in APP^{swe}/PSEN1^{dE9} (APP/PS1) mice, an animal model of AD, because of increased activity in compensatory genes for a GABA-synthesizing enzyme, diamine oxidase (DAO). We have developed a potent, highly selective, and reversible MAO-B inhibitor, KDS2010 (IC₅₀: 7.6 nM; 12,500-fold selectivity over MAO-A), which overcomes the disadvantages of the irreversible MAO-B inhibitor. Long-term treatment with KDS2010 does not induce the compensatory mechanisms, thereby significantly attenuating increased astrocytic GABA levels and astrogliosis, enhancing synaptic transmission, and rescuing learning and memory impairments in APP/PS1 mice.

Poster Presentation : **MEDLP-408**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

A Retro-biosynthetic Accelerated Approach to Finding Novel Synthetic Scaffolds of Hit to Lead Compounds

Tara Man Kadayat, Sung Jin Cho*, Jungwook Chin*

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

(Marine) Natural products have long been providing a reasonable ground for uncharted drug discovery. However, due to their intricate molecular frameworks and unexplored chemical synthetic arena, the access to secure them in an economically sound method through semi-synthesis, total synthesis or isolation is often fraught with difficulties. Herein, this study aims to provide a potential solution with respect to scale and concise chemical synthesis through the logic of “Retro-Biosynthetic Accelerated Approach”. Starting from the economically viable secondary metabolites or natural sources from micro/macro organisms that pertain privileged scaffolds, the adoption of well-established synthetic/biosynthetic methods could yield libraries of ‘high value’ drug-like lead compounds. This method easily extends on the conventional process of the drug discovery, such as identifying hit compounds to early stage of lead compounds, and new scientific findings are warranted.

Poster Presentation : **MEDIP-409**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Diastereoselective Synthesis of 1-Aminoindanes via Rhodium(III) Catalyzed C-H Activation

Heeyoung Lee, Daeun Jeung, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

Indane has been recognized as an important structural motif in organic synthesis and medicinal chemistry. Particularly, 1-aminoindanes have attracted considerable attention by virtue of their interesting biological properties, such as anti-inflammatory, analgesic, antipyretic, anticonvulsant, anti-leukemic, anti-Parkinson and etc. Therefore, a range of 1-aminoindane derivatives have been synthesized and evaluated for their clinical applications. In this context, imine directing groups have been widely used for new C–C bond formation reactions with various unsaturates such as alkenes, alkynes, and allenes. Additionally, Re(I) and Ru(II) catalysts were also employed in C–H functionalization of ketimines with alkynes and allenes to deliver the corresponding 1-aminoindenes and 1-aminoindanes, respectively. Moreover, Nishimura disclosed the Ir(I)-catalyzed stereoselective annulation of cyclic N-sulfonyl and N-acyl ketimines with 1,3-dienes to yield spiroaminoindane derivatives. Despite of great progress on the coupling reaction between imines and π -unsaturates, examples of annulation reaction using internal alkenes with high diastereoselectivity are still unexplored. In continuation of our recent works on the catalytic sp² and sp³ C–H functionalizations using internal olefins including maleimides, we herein describe the Rh(III)-catalyzed diastereoselective formation of 1-aminoindanes using N-sulfonyl aldimines and various olefins.

Poster Presentation : **MEDLP-410**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

The reactivity of MBH adducts with benzylamines to access the 2-benzazepines under Rh(III) catalysis

Neeraj kumar Mishra, Prithwish Ghosh, Won An, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

The directing group assisted transition-metal-catalyzed C–H activation has been one of the most attractive issues in organic synthesis due to their site selective C–H bond functionalization, easy to remove after reaction and undergo annulation reaction to offered new biologically active heterocyclic scaffolds. In this addition, free NH₂ group as a directing group is less explored because of its poisoning nature for the transition-metal. The Morita–Baylis–Hillman adduct (MBH) has been recognized as a useful 3-carbon synthon in C–C bond formation reactions. Azepine analogues are among the most interesting discovery in the field of natural products and pharmaceuticals. Particularly, benzazepine derivatives have attracted considerable attention by virtue of their interesting biological properties. Typical examples, such as galanthamine, capsazepine, and baclabuvir include the 2-benzazepine scaffold. Therefore, the synthesis of 2-benzazepines is of great interest in organic and medicinal chemistry. In this presentation, the rhodium(III)-catalyzed cross-coupling reaction between commercially available benzylamines and Morita–Baylis–Hillman adducts is described. This protocol provides a facile route for synthesis of various 2-benzazepine derivatives via C(sp²)-H activation of in situ generated N-allyl benzylamines from MBH adduct and subsequent intramolecular olefin insertion process. To gain mechanistic insight of this transformation, DFT calculations were also performed.

Poster Presentation : **MEDIP-411**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Ginsenoside Rb2 suppresses the glutamate-mediated oxidative stress and neuronal cell death in HT22 cells

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Natural Products Research, Korea Institute of Science and Technology, Korea

¹*Convergence Research Center for Diagnosis, Treatme, Korea Institute of Science and Technology, Korea*

²*Department of Dentistry, Gangneung-Wonju National University, Korea*

³*Korea Institute of Science and Technology, Korea*

⁴*Convergence Research Center for Dementia DTC, Korea Institute of Science and Technology, Korea*

Background: The objective of our study was to analyze the neuroprotective effects of ginsenoside derivatives, Rb1, Rb2, Rc, Rd, Rg1, and Rg3 against glutamate-mediated neurotoxicity in HT22 hippocampal mouse neuron cells. Methods: The neuroprotective effect of ginsenosides were evaluated by measuring cell viability. Protein expression of mitogen-activated protein kinase (MAPK), Bcl2, Bax, and apoptosis inducing factor (AIF) were determined by western blot analysis. The occurrence of apoptotic and death cells were determined by flow cytometry. Cellular level of Ca²⁺ and reactive oxygen species (ROS) levels were evaluated by image analysis using the fluorescent probes Fluor-3 and 2',7'-dichlorodihydrofluorescein diacetate (DCF₂DA), respectively. In vivo efficacy of neuroprotection was evaluated using the Mongolian gerbil of ischemic brain injury model. Result: Reduction of cell viability by glutamate (5 mM) was significantly suppressed by treatment with ginsenoside Rb2. Phosphorylation of MAPKs, Bax, and nuclear AIF was gradually increased by treatment with 5 mM of glutamate and decreased by co-treatment with Rb2. The occurrence of apoptotic cells was decreased by treatment with Rb2 (25.7 μ M). Cellular Ca²⁺ and ROS levels were decreased in the presence of Rb2, and in vivo data indicated that Rb2 treatment (10 mg/kg) significantly diminished the number of degenerated neurons. Conclusion: Our results suggest that Rb2 possesses neuroprotective properties that suppress glutamate-induced neurotoxicity. The molecular mechanism of Rb2 is by suppressing the MAPKs activity and AIF translocation.

Poster Presentation : **MEDIP-412**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

C-H Aminocarbonylation of N-(Hetero)aryl-7-azaindoles with Isocyanate under Ruthenium(II) Catalysis

Taejoo Jeong, Kunyoung Kim, Na Yeon Kwon, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

7-Azaindoles as bioisosteres of indoles have been known to display diverse biological profiles. With great advances in organic and medicinal chemistry, a number of 7-azaindoles have been synthesized and screened for clinical trial. For examples, vemurafenib (Zelboraf™), decernotinib, PLX647, GSK1070916, and BMS378806, are currently on the market or under clinical phase. In this context, the directing group-assisted C-H functionalization of 7-azaindoles has been recognized as the useful strategy to generate the highly substituted 7-azaindole derivatives. However, to our best knowledge, the Ru(II)-catalyzed 7-azaindole-directed C-H aminocarbonylation has been unexplored. In our recent studies on the synthesis of biologically active compounds based on catalytic C-H functionalization, we herein disclose the site-selective Ru(II)-catalyzed C-H aminocarbonylation of 7-azaindoles with alkyl and aryl isocyanates to afford the corresponding ortho-amidated 7-azaindoles.

Poster Presentation : **MEDIP-413**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

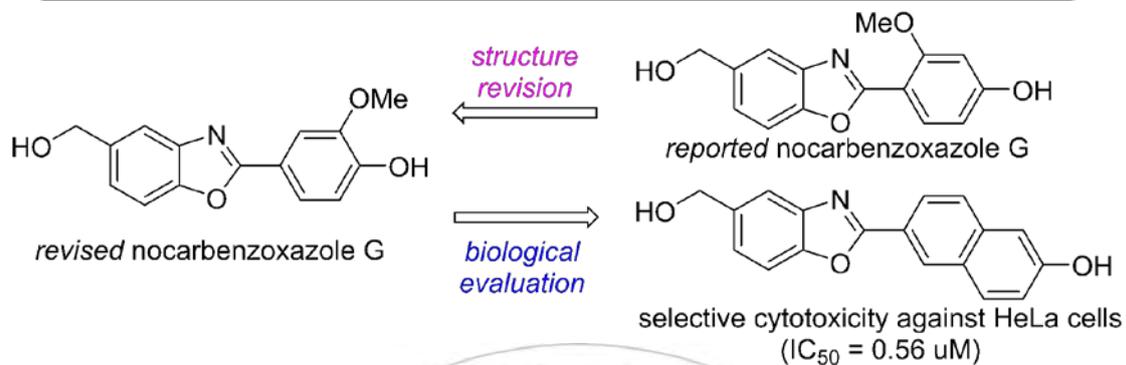
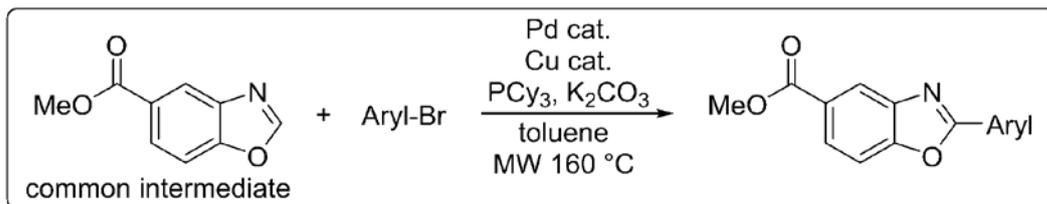
Synthesis, Structure Revision, and Biological Evaluation of Nocarbenzoxazoles

Young seok Kim, Taejung Kim¹, Jungyeob Ham^{1,*}

Gangneung-Wonju National University, Korea

¹*Natural Products Research, Korea Institute of Science and Technology, Korea*

The total synthesis of nocarbenzoxazoles F and G, obtained from the marine-derived halophilic strain *Nocardiopsis lucentensis* DSM 44048, was achieved via a simple and versatile route involving microwave-assisted construction of a benzoxazole skeleton, followed by carbon-carbon bond formation with the corresponding aryl bromides. Unfortunately, the ¹H and ¹³C NMR spectra of natural nocarbenzoxazole G did not agree with those of the synthesized compound. In particular, the spectra of the isolated and synthesized compounds showed considerable differences in the signals from the protons and carbons in the aryl group. The revised structure was validated by the total synthesis of the actual nocarbenzoxazole G molecule, which is a regioisomer of the compound that was reported earlier as nocarbenzoxazole G. The synthesized derivatives showed specific cytotoxicity to the human cervical carcinoma cell line, HeLa, but did not have any remarkable effect on the other cell lines.



Poster Presentation : **MEDIP-414**

Medicinal Chemistry

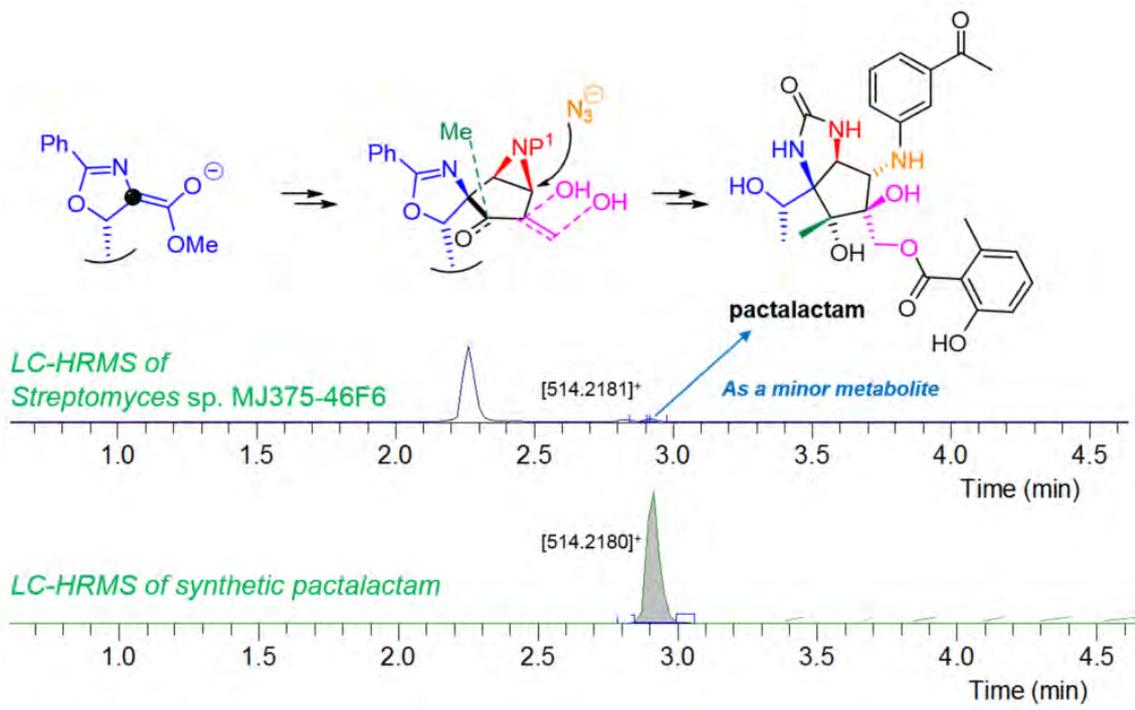
Exhibition Hall 2, THU 11:00~12:30

Total Synthesis of Pactalactam, a Cyclic Urea Analog of Pactamycin

Taejung Kim, Young-Tae Park, Jungyeob Ham*

Natural Products Research, Korea Institute of Science and Technology, Korea

Pactalactam, with a densely functionalized aminocyclopentitol core featuring six contiguous stereogenic centers, was isolated from a fermentation broth of *Streptomyces pactum* var. *pactum* as a minor component in 1980. Pactamycin, a major component of the above culture broth, has a wide range of biologically attractive properties and a unique chemical structure. However, its development as a clinical drug was curtailed due to its broad and potent cytotoxicity. Therefore, the synthesis of pactalactam a cyclic urea pactamycin analog, has focused on the development of new synthetic strategy, and securing biological research data and chemical information. The cyclopentane framework was obtained by means of ring-closing metathesis (RCM) and aldol coupling with L-threonine-derived optically active oxazoline. The key steps were the substrate-controlled stereoselective aziridination and the regioselective aziridine ring-opening by azide for the construction of three-continuous amino groups, face-selective dihydroxylation, and addition of methyl anion on the octa-substituted cyclopentane core. Finally, reductive oxazoline ring-opening reaction, construction of the cyclic urea moiety, 3-acetylphenyl group introduction by Cu-catalyzed C-N bond formation, primary alcohol-selective acylation and sequential deprotection gave reported structure of pactalactam. Furthermore, the existence of pactalactam in culture broth of pactamycin-producing *Streptomyces* sp. was revealed by comparison of synthetic sample.



Poster Presentation : **MEDIP-415**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Discovery of Imidazopyridine Derivatives as Type II Inhibitors of the T315I Mutant BCR-ABL-Target

Ye Ri Han, Doohyun Lee, Chunyoung Im*

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

Chronic myeloid leukemia (CML) is a type of cancer caused by the translocation between ABL1 gene in chromosome 9 and the BCR gene in chromosome. This translocation leads to the formation of fusion protein BCR-ABL which are constitutively active tyrosine kinase that induces the pathogenesis of CML. Despite the presence of several well-known inhibitors such as imatinib, Bcr-Abl tyrosine-kinase inhibitors are still receiving significant interest due to the tolerance by the T315I mutation. Therefore, it is important to discover new T315I-mutant BCR-ABL-target inhibitors. Here we describe a imidazopyridine-based type II inhibitors which are targeting T315I-mutated BCR-ABL. The compounds showed significant in vitro efficacy against BCR-ABL-T315I as well as BCR-ABL-WT. In addition, pharmacokinetic data and DMPK profile displayed that the several resulting compounds have optimal ADME properties. Thus, the imidazopyridine-based compounds which are synthesized in this study will be further investigated for the development of a new target treatment for CML.

Poster Presentation : **MEDIP-416**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

The change of ginsenosides composition in ginseng leaves extract by the microwave-processed

Bong Geun Song, Pilju Choi¹, Chulhee Yoon, Sang Il Jeon, Jungyeob Ham^{1,*}

Department of Chemistry, Gangneung-Wonju National University, Korea

¹Natural Products Research, Korea Institute of Science and Technology, Korea

Ginsenosides are the main active constituents in *Panax ginseng*, and the main ginsenosides can be derived from every part of the plant. More than 30 ginsenosides have been isolated from *Panax ginseng*, most of which contain one of 4 aglycone moieties. However, several studies on the ginsenoside contents of the other parts of *Panax ginseng* have been reported, and there are some studies on the variation of ginsenoside structures in different parts of the *Panax* species. Although the most commonly used parts of ginseng are the roots and rhizomes, ginsenosides are also present in the aerial parts of *Panax* species. However, the underground and aerial parts generally show different ginsenoside profiles. The components and pharmacological properties of ginseng leaf are not completely understood. More interestingly, some reports indicate that the content of active components in the leaf is higher than that in the root. In this study, we propose a microwave processing method of ginseng leaves to increase the contents of ginsenoside Rg6, Rk3, Rh4. The ginsenosides Rg6, Rk3 and Rh4 were not detected in the ginseng leaf extracts, but microwave-processed method of ginseng leaf extract to be included their contents were 16.5, 26.7, and 30.0 mg respectively.

Poster Presentation : **MEDIP-417**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

A novel cereblon modulator for targeted protein degradation

**Hyung Soo Kim, Jong Yeon Hwang^{1,*}, Jae du Ha², Sung Yun Cho², Pilho Kim¹, AhRa Go¹,
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³*pharmacy, Sungkyunkwan University, Korea*

Immunomodulatory drugs (IMiDs) exert anti-myeloma activity by binding to the protein cereblon(CRBN) and subsequently degrading IKZF1/3. We design and synthesize a novel IMiD analog TD-106 that induces the degradation of IKZF1/3 and inhibits the proliferation of multiple myeloma cells in vitro as well as in vivo. These results, therefore, firmly suggest that the newly synthesized IMiD analog, TD-106, is a novel CRBN modulator that can be used for targeted protein degradation.

Poster Presentation : **MEDIP-418**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and recent updates on thiazoline containing agonists of selective peroxisome proliferator-activated receptor δ

Tara Man Kadayat, Su-Jeong Lee, Sung Jin Cho*, Jungwook Chin*

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

Peroxisome proliferator-activated receptors (PPARs) are members of ligand-activated transcription factors of the nuclear receptor family. Based on distinct ligand specificity, physiological roles and tissue distribution, PPARs are classified into three isotypes namely PPAR α , PPAR γ , and PPAR δ . PPAR δ is considered as a promising biological target for the development of new drugs to treat metabolic syndrome including hyperlipidemia. As part of our continuous effort to develop new analogues of GW501516 (a well-known selective and potent PPAR δ agonist), we introduced a facile method for the synthesis of new thiazoline containing intermediate for the preparation of novel PPAR δ -selective agonists. The synthetic method used is short and convenient as it did not require the use of extreme conditions such as -78 °C. In this study, we developed efficient route for the synthesis of distinctive thiazoline containing compounds as selective PPAR δ agonists. These reaction conditions and unique key intermediate may be applicable for the synthesis of other related pharmaceuticals. The preliminary in vitro PPAR δ activity of synthesized compounds demonstrates this unique thiazoline core containing compounds as potential PPAR δ -selective agonist. In addition to this synthetic work, recent updates on selective agonists of PPAR δ will also be described.

Poster Presentation : **MEDIP-419**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

The Development and lead Optimization of Transglutaminase 2 Inhibitors for the Treatment of Renal Cell Carcinoma (RCC).

**Eun Bi Ko, Chunyoung Im, Ga Young Park, JiHee Kang, Eunhye Lee, Soong-Hyun Kim,
Minsoo Song***

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

Renal cell carcinoma (RCC) is the most common malignant tumor of the human kidney. In RCC cell lines, Transglutaminase 2 (TGase 2, E.C. 2.1.2.13), a protein cross-linking enzyme, is considerably over-expressed in comparison to the level of TGase 2 expression in normal kidney. TGase 2 in RCC binds directly to p53 and induces p53 depletion by the process of autophagy, consequently RCC surviving from p53-induced apoptosis. Therefore, hindering RCC growth via inhibition of TGase 2 could be an effective strategy to treat RCC. In order to develop new inhibitors of TGase 2, we designed small molecule inhibitors of TGase 2. Over 250 compounds were synthesized and the biological activity of the compounds was determined by in vitro enzyme assay and cell-based assay. Through our SAR analysis, several compounds are identified as highly potent TGase 2 inhibitors. Series of compounds were selected for ADME/T test and xenograft experiments. As a result, we have found compound DN201782 as a lead compound with in vitro and in vivo efficacy. That could be applied to potential therapeutic agent for treating RCC. Herein, experimental data and xenograft results are presented in detail.

Poster Presentation : **MEDIP-420**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Pyrrolo[2,3-D] Pyrimidine derivatives, A Cathepsin K Inhibitor for The Treatment of Osteoporosis

Jusuk Lee, Ji Hoon Lee*

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

Osteoporosis is a disease where increased bone weakness increases the risk of a broken bone. When bone resorption exceeds bone formation, pathologic processes, such as osteoporosis, can result. Cathepsin K, a lysosomal cysteine protease that is expressed by osteoclasts during the process of bone resorption, acts as the major collagenase responsible for the degradation of the organic bone matrix during the bone remodeling process. Because excessive bone remodeling is a key element in the pathogenesis of postmenopausal osteoporosis and other skeletal disorders, cathepsin K is a potential target for therapeutic intervention. In order to develop new inhibitors of Cathepsin K, we synthesized a series of pyrrolo [2,3-D] pyrimidine derivatives and evaluated their in vitro cathepsin K inhibitory activity. The screening results show that the potency of most compounds were equal to or greater than that of the reference compound. Finally, we found pyrrolo [2,3-D] pyrimidine structure as highly potent Cathepsin K inhibitor.

Poster Presentation : **MED.P-421**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Studies of secondary metabolites isolated from Korean mushroom

Seon-Jun Choi, Young Seok Kim¹, Sang Il Jeon¹, Jungyeob Ham*

Natural Products Research, Korea Institute of Science and Technology, Korea

¹Department of Chemistry, Gangneung-Wonju National University, Korea

To investigate the biological activity of various natural products derived from mushrooms, this study selected *Suillus granulatus* of Gangwon-do wild mushrooms, isolated the components and studied its chemical structure and biological activity. The methanol extract of *Suillus granulatus* was fractionated according to the polarity, and the ethyl acetate layer was selected and divided by reverse phase column and size exclusion chromatography. Suillusin and new substance suillusin B and C were isolated from M2 fraction. Suillusin had an insufficient effect on biological activity in the previous reports, and it is an edible mushroom that has lower toxicity. As a result of measurement of a new activity on lung cancer metastasis, it had an inhibitory effect on the EMT phenomenon of lung cancer cell (A546 cell) by TGF beta. As a result of measurement of the activities of suillusin B and suillusin C, too, their cytotoxicity was low, and the inhibitory effect on lung cancer metastasis was higher in suillusin B than suillusin and suillusin C. *Suillus granulatus* had an inhibitory effect on lung cancer metastasis as an edible mushroom with low cytotoxicity. It is expected that it would have a less side effect and wider value of use since it has low cytotoxicity.

Poster Presentation : **MEDIP-422**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development and Lead optimization of CETP inhibitors for cardiovascular diseases

Eunhye Lee, Soong-Hyun Kim, Ga Young Park, Eun Bi Ko, Chunyoung Im, Minsoo Song*

*New Drug Development Center (NDDC), Daegu-Gyeongbuk Medical Innovation Foundation (DGMIF),
Korea*

Cholesteryl ester transfer protein (CETP) is a plasma glycoprotein which catalyzes a mutual exchange of cholesteryl esters (CEs) and triglycerides (TGs) among lipoproteins such as high density lipoprotein (HDL), low density lipoprotein (LDL), and very low density lipoprotein (VLDL). Physiological role of CETP is to transfer CEs from HDL to LDL/VLDL in exchange for TGs, consequently decreasing HDL-C levels and increasing LDL-C levels in plasma. Such event by CETP in plasma might be proatherogenic based upon epidemiological studies and therefore, inhibition of CETP could be a potential therapy to reduce atherosclerotic cardiovascular disease (ASCVD) risk. Accordingly, CETP has been targeted intensively in drug-development society especially by major pharmaceutical companies, and the most advanced study has been on anacetrapib from Merck with successful efficacy in clinical trial phase III. Recently, we designed a novel series of small molecules as CETP inhibitor for ASCVD and over 150 compounds were synthesized. In vitro CETP inhibitory activity of each compound was obtained by single dose (80nM) treatment of inhibitor using commercially available assay kit. Several compounds were highly potent and tested for ADME/T assay and rodent PK experiments. Our lead compound showed comparable efficacy to anacetrapib both in vitro and in vivo. Efficacy dose of the lead compound was determined based on mouse PK data and subjected to in vivo efficacy experiment using hCETP/ApoB dual transgenic mice. One month-period of efficacy test with 4 animal groups (anacetrapib vs DN201929) was executed. Analysis of the efficacy data of HDL/LDL levels and histopathologic examination provided promising results. Detailed experimental and efficacy data are presented in this poster.

Poster Presentation : **MEDIP-423**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development of fluorescent probe SiR-Mito11 targeting mitochondria for cancer treatment and diagnosis

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²*Department of Molecular Science and Technology, Ajou University, Korea*

Mitochondria is an important cellular organelles not only for energy metabolism by APT synthesis, but also for ROS production and consequent cell death signaling. Due to the important role of mitochondria in oncogenesis and tumor anabolism, mitochondria has been considered as a target for anti-cancer agent. Therefore, mitochondria can be used as a biological marker for selectively treating and diagnosing cancer. When the theragnosis is in the spotlight in these days, it is possible to target the mitochondria for theragnosis approach. In previous paper, we developed NIR-fluorescent probe SiR-Mito8 that targets mitochondria specifically. However, undesired cytotoxicity was observed in normal cells. To enhance cellular specificity, we developed SiR-Mito11 that acts more selectively in a cancer cell by tuning hydrophobicity of compound. We demonstrated that SiR-Mito11-induced cellular toxicity was particularly selective in neuroblastoma compared to neuron cells. Therefore, We confirmed a potential ability of SiR-Mito11 for cancer specific therapeutic and diagnostic probe.

Poster Presentation : **MEDIP-424**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Tetrahydroisoxazolopyridine, Benzisoxazol and Pyridoindole Derivatives as 5-HT₆ Receptor Antagonists

Young Jin Choi, Hyunah Choo^{1,*}, Ghilsoo Nam^{1,*}

Division of Bio-Med, University of Science & Technology, Korea

¹*Korea Institute of Science and Technology, Korea*

Serotonin is a neurotransmitter with a monoamine structure that biosynthesized from tryptophan, also is known as 5-hydroxytryptamine (5-HT). The Serotonin does not pass easily through the BBB (Blood Brain Barrier), so it is serotonin biosynthesized after passing through the brain wall with tryptophan or 5-hydroxytryptophan. Serotonin plays a role in activating brain-regulated sleep, appetite, libido, pain, and biorhythm. It also associated with mental disorders such as depression, anxiety, schizophrenia, obsessive compulsive disorder, panic disorder, obesity. The 5-HT receptor that binds to serotonin is the GPCR, which has seven transmembrane domains, three extracellular loops, and three intracellular loops. The 5-HT receptor has 14 subtypes (5-HT_{1a} to 5-HT₇) according to the second messenger. Among them, 5-HT₆ was discovered in 1993, and recently 5-HT₆ has actively studied as good drug targets such as obesity, sleep, cognitive impairments. AD (Alzheimer Disease) is most common in people with dementia, but there is currently no cure. 5-HT₆ is a good target of reduced side effects due to the 5-HT₆ is mainly distributed in the CNS and rarely existed in the PNS. Here we present the design and synthesis of a series of tetrahydroisoxazolopyridine derivatives a various substituted HYD (Hydrogen Donating) groups, and pyridoindole derivatives having various HBA (Hydrogen Bond Accepting) groups in detail.

Poster Presentation : **MEDIP-425**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of derivatives as transthyretin (TTR) kinetic stabilizer that can inhibit amyloidosis.

SeoYun Kim, Eunhee Jeon, Yunlan Kim, Sungwook Choi*

Development of Drug Development and Discovery, Chungnam National University, Korea

Transthyretin (TTR) is a homo-tetrameric protein composed of 127-amino-acid, β -sheet-rich subunits. The physiological functions of TTR are to bind and to transport the thyroid hormone thyroxine (T₄) and holoretinol binding protein in the blood and cerebrospinal fluid (CSF). However, aggregation of TTR or mutant TTR are leads to human amyloid diseases such as Senile Systemic Amyloidosis (SSA), Familial Amyloid Cardiomyopathy (FAC), Familial Amyloid Polyneuropathy (FAP). Thus, small molecule as the kinetic stabilizer is used to prevent TTR amyloidosis-related diseases. small molecule that binds to T₄ binding site stabilize the ground state of tetrameric TTR and raise the kinetic barrier for tetramer dissociation, imposing kinetic stabilization on TTR and preventing aggregation. As examples of stabilizers for small molecules, Tafamidis (Vyndaqel) was approved by the European Medicines Agency (EMA) in 2011 and in Japan in 2013 for the treatment of transthyretin cardiomyopathy and AG10 showed good activity against TTR aggregation inhibition. Therefore, we synthesized derivatives that bind to T₄-binding sites within TTR tetramer using Structure-Based Drug Design (SBDD).

Poster Presentation : **MEDIP-426**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Rh(III)-Catalyzed Synthesis of N-Heterocyclic Fluorescent Materials as Bioimaging Agent

Sangbong Lee, Ye Ri Han, Jungwook Chin, Su-Jeong Lee, Sung Jin Cho*, Dong-Su Kim*

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

Synthesis of N-heterocyclic compounds using Rh(III) catalysis received great attentions in various fields of study such as pharmaceutical and materials area. Recently, we also reported synthesis of N-heterocyclic compounds as pyridine and isoquinoline using allylamine and benzylamine in the presence of Rh(III)/Cu(II) complex. During the course of our studies, new efficient synthetic method for the synthesis of N-heterocyclic salt compounds was developed. Interestingly, their fluorescent spectra showed over the full color region. Based on these previous studies, we attempted for application of fluorescent materials to diagnostic bioimaging in vivo model. For successful application of fluorescent materials as imaging agent, several in vitro and in vivo experiments were performed. We initially examined cytotoxicity of fluorescent materials in various cell lines such as normal fibroblast cells (BJ6) and macrophage to show no difference between untreated and treated cells at various doses. Next, in vivo fluorescent imaging studies were achieved to demonstrate the ability of these imaging agents for specific target disease. As a result, we found that benzoquinolizinium salt can be employed to serve as an in vivo imaging agent for detection of imflamed lesions. This result is possible to be applied to diagnosis of disease.

Poster Presentation : **MEDIP-427**

Medicinal Chemistry

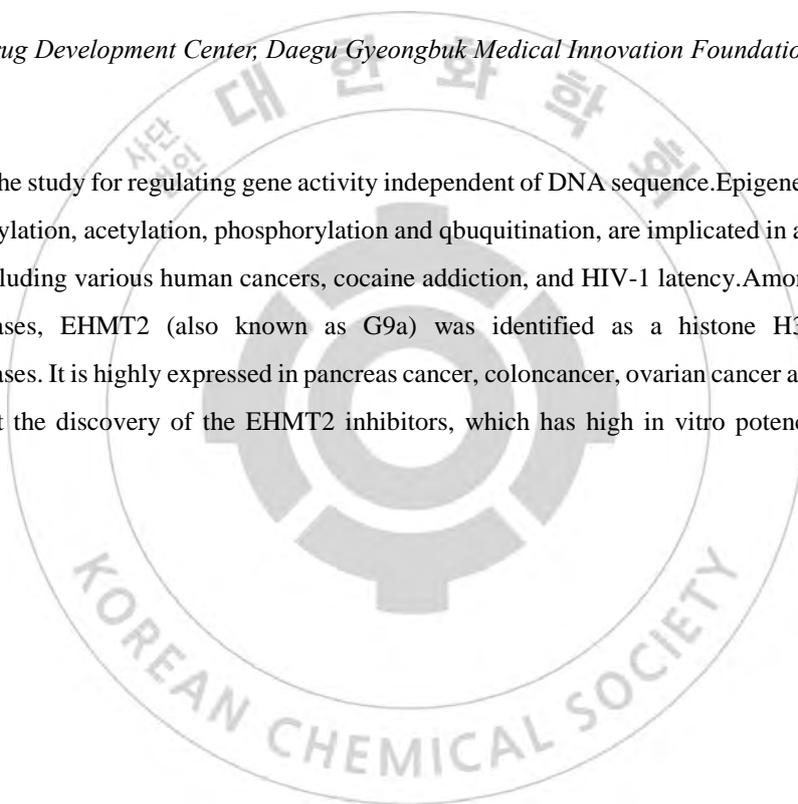
Exhibition Hall 2, THU 11:00~12:30

Discovery of potent and selective inhibitors for EHMT2(G9a)

Sugyeong Kwon, Na Yeon Kim, Jina Kim, Shinae Kim*

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

Epigenetics is the study for regulating gene activity independent of DNA sequence. Epigenetic modifications, including methylation, acetylation, phosphorylation and ubiquitination, are implicated in a broad spectrum of diseases, including various human cancers, cocaine addiction, and HIV-1 latency. Among protein lysine methyltransferases, EHMT2 (also known as G9a) was identified as a histone H3 Lys9 (H3K9) methyltransferase. It is highly expressed in pancreas cancer, colon cancer, ovarian cancer and breast cancer. Here we report the discovery of the EHMT2 inhibitors, which has high in vitro potency and excellent selectivity.



Poster Presentation : **MEDIP-428**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of thiophene-acylguanidine derivatives and evaluation of nematicidal activity

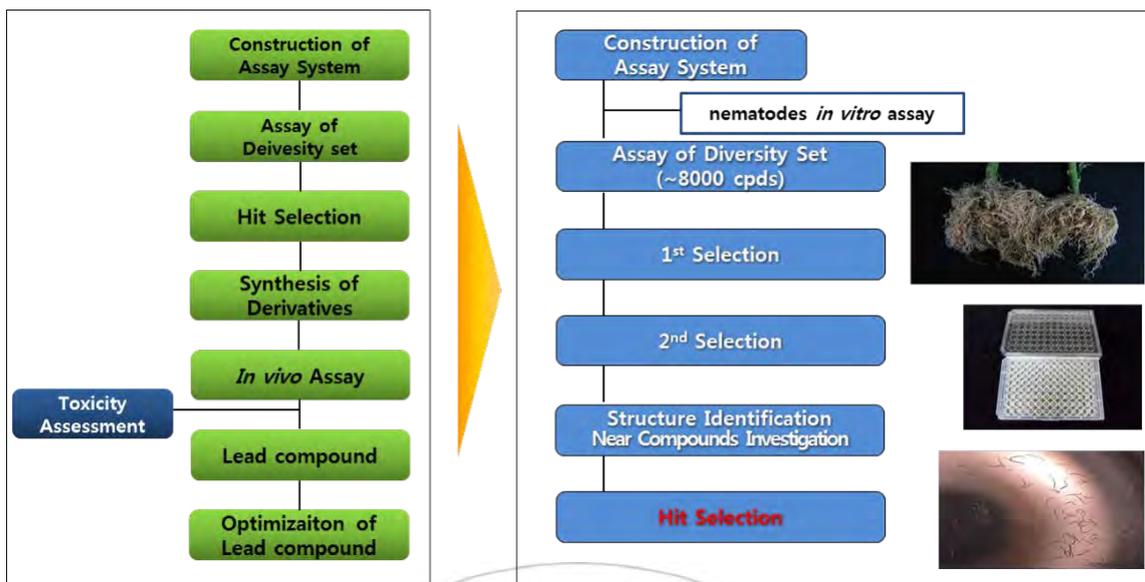
Solbin Kim, Hyun Suk Yeom^{1,*}, ChangJu Yoon²

Chemistry, Hanyang University, Korea

¹*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

²*Chemistry, Sungkyunkwan University, Korea*

The resulting record of less-than-perfect environmental or human health safety has resulted in the widespread deregistration of several agronomically important nematicides. The organophosphates, carbamates, and fumigants, which have been traditionally used, are increasingly restricted due to environmental and toxic problems. Therefore, there is a constant demand for the development of a novel nematocide that exhibits a broad nematode control spectrum at low application rates as a solution to problems such as impact on the human health and global environment. Recently, we have discovered several hits with nematicidal activity against *M. incognita* through assay of chemical library (~8000 cpds) from Korea Chemical Bank in KRICT. Among them, the compound having thiophene-acylguanidine moiety showed excellent nematicidal activity even at 5 ppm level. In the field of medicinal chemistry, the physiological activity results for many compounds including acylguanidines have already been reported and are known as the important pharmaceutical core of the NHE-1 inhibitor, particularly in relation to cardio-protection therapy. However, little research has been done on compounds containing acyl guanidines as agrochemical. At this presentation, the process of selecting new hits and structure-activity relationship(SAR) between acyl guanidine derivatives and nematicidal activity will be discussed briefly.



Poster Presentation : **MEDIP-429**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Efficient synthetic methods of 7-trifluoromethyl-7-deazapurine ribonucleoside analogs and their phosphoramidate prodrugs

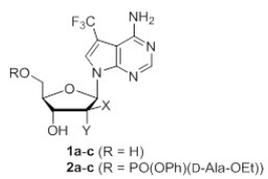
Jong Hyun Cho^{*}, Franck Amblard¹, Leda C. Bassit¹, Steven J. Coats², Raymond F. Schinazi¹, SeMyeong Choi

Dong-A University, Korea

¹*Emory University, United States*

²*Co-crystal Pharma, United States*

New 7-trifluoromethyl-7-deazapurine ribonucleoside analogs (**1a-c**) and their Prodrugs (**2a-c**) were successfully synthesized from riborlactol and 1- α -bromo-ribose derivatives using Silyl-Hilbert-Johnson or nucleobase-anion substitution reaction and then aromatic trifluoromethyl substitution as key step reactions. The β -selective glycosylation reaction of the benzyloxonium ribose, or 1- α -bromo-ribose intermediates with persilylated 6-chloro-7-iodo-7-deazapurine, or anionized compound, followed by the aromatic trifluoromethylation reaction with MFSDA and CuI and then treatment with ammonia afforded 7-trifluoromethyl-7-deazapurine ribonucleosides (**1a-c**) in excellent yield, which were converted into their phosphoramidate prodrugs (**2a-c**) employing chlorophosphoramidate derivative. Unfortunately, all of them showed no potent anti-HCV, anti-Zika and anti-Ebola activities with cytotoxicity.



Poster Presentation : **MEDIP-430**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Identification of novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

Jiwoong Lim, Ae Nim Pae^{1,*}, Jae Wook Lee², Sang Min Lim¹, Jae Yeol Lee³

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³*Department of Chemistry, Kyung Hee University, Korea*

SHIP2 domain-containing inositol 5'-phosphatase 2 (SHIP2) is a lipid phosphatase that produce phosphatidylinositol 3,4-bisphosphate (PI(3,4)P₂) from phosphatidylinositol 3,4,5-triphosphate (PI(3,4,5)P₃), and is involved in various human diseases including type 2 diabetes, cancer, and neurodegenerative diseases. A recent report demonstrated that inhibition of SHIP2 leads to functional restoration of the Akt/GSK3-dependent pathway by reducing the levels of PI(3,4)P₂. Furthermore, the fact that downregulation of the SHIP2 reduced tau hyperphosphorylation induced by amyloid β and rescued the memory impairment in a Alzheimer's disease mouse model indicates SHIP2 can be a promising therapeutic target for Alzheimer's disease. In this study, we have developed novel, potent SHIP2 inhibitors by extensive structural elaboration of hit compounds discovered from a high-throughput screening. The biological evaluation revealed that some of the synthesized compounds had good potency on SHIP2 inhibition with reasonable drug-like properties in comparison with reference compounds. Notably, one of these derivatives, compound 43, showed promising properties in an in vivo pharmacokinetic evaluation and BBB penetration study. Considering SHIP2 is one of key signal mediators for tau hyperphosphorylation, our potent SHIP2 inhibitor may function as a promising lead compound for the treatment of Alzheimer's disease.

Poster Presentation : **MEDIP-431**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis of Ascorbyl Conjugated Peptide Derivatives and Evaluation of Collagen Stimulating Activity in Human Skin Fibroblasts

Jiyeon Kim, Jun Goo Kang¹, Taek Jin Kim¹, Kyeong yong Park^{1,*}

Biomedical Laboratory Science, Eulji University, Korea

¹*Integrated Materials Development, Chameditech, Korea*

Vitamin C is an widely used agent for anti-aging and whitening in the field of cosmetics which has effects in collagen production of skin cells, inhibition of melanin synthesis, anti-oxidant activity, and improvement of immune system. However, since vitamin C has many problems in cell permeability and stability derived from environment condition such as heating and lighting, its derivatives are being developed to overcome these problem. In this study, we synthesized vitamin C derivatives with succinoyl group at 2-position and peptides in the form of ester bond and its cytotoxicity and collagen synthesis activity were evaluated in human skin fibroblasts. In addition, vitamin C-peptide were synthesized in ether and carbamate form, and the optimal combination of vitamin C and peptides was identified. The activity of collagen synthesis was also evaluated and compared with that of vitamin C.

Poster Presentation : **MEDI.P-432**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Identification and structure analysis of antimicrobial materials from natural biological resources that were collected from southeast asian countries

Yeseul Park, Dong-Ku Kang^{1,*}

Chemistry, Incheon National University, Korea

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

This study aims to develop the antimicrobial materials from natural biological resources that were collected from southeast asian countries including Vietnam, Cambodia, Myanmar or Thailand. Natural plant resources were collected by Korea National Institute of Biological Resources (KNIBR) and then extracted samples were supplied for the screening of antimicrobial activity at Incheon National University. First, dried samples were homogenized and extracted with 70% ethanol. Antimicrobial activities of one hundred whole extracts were identified using conventional paper disc assay against infectious pathogens such as *Escherichia coli* (gram negative), *Staphylococcus aureus* (gram positive), *Proteus mirabilis* (gram negative), *Streptococcus pseudopneumoniae* (gram positive), and *Candida albicans* (yeast). Then, quantitative assay of antimicrobial activity was performed to validate the IC₅₀ values on 1st selected samples using alamarBlue-based cell viability assay. Sample No.85 was found to have excellent antimicrobial activity in *S. aureus* and *S. pseudopneumoniae* strains on paper disc assay. The IC₅₀ value of No.85 was identified as 0.073 mg/ml against *S. aureus* and 0.005 mg/ml against *S. pseudopneumoniae*. While the IC₅₀ of gentamicin, a positive control, was 2.167 mg/ml and 1.181 mg/ml, respectively in *S. aureus* and *S. pseudopneumoniae*. Then, fractionation was carried out by HPLC and the antimicrobial activity was identified to define active chemical compound from each fractions. The structure of chemical compounds were determined by NMR and Mass spectrometry.

Poster Presentation : **MEDIP-433**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Anti-oxidant Effects of Secondary Metabolites from the Marine Fungus *Penicillium* sp. 168CLC-17.1

Byeoung-kyu Choi, Phan Thi Hoai Trinh¹, Tran Thi Thanh Van¹, Hee Jae Shin*

*Marine Natural Products Chemistry Laboratory, Korea Institute of Ocean Science & Technology, Korea /
Department of Marine Biotechnology, University of Science and Technology, Korea*

¹*Nhatrang Institute of Technology Research and Application, Vietnam Academy of Science and
Technology, Vietnam*

The marine environment has played a significant reservoir of natural products for new drugs over the last few decades. The majority of novel secondary metabolites from the ocean have structural diversities and potent bioactivities. Marine-derived microorganisms, especially marine fungi, are considered as a novel source in the biological and chemical fields. Moreover, many natural products from marine fungi were developed as medicines and are being studied to cure diverse diseases and infections. The fungus 168CLC-17.1 was isolated from a sediment sample, collected at Cu Lao Cham island, Quang Nam, Vietnam by modified Sabouraud medium and identified as *Penicillium janthinellum*. From the strain, a p-terphenyl derivative, emodin and aflavinin were isolated from the EtOAc extract. Their structures were determined by MS, 1D and 2D NMR data analyses. All compounds were tested for anti-oxidant capacities using ABTS, DPPH and ORAC assays. Among them, 3,3'-dihydroxy-6'-desmethylterphenyllin (1) showed potent anti-oxidant activities.

Poster Presentation : **MEDIP-434**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Development and identification of biocompatible antimicrobial materials from endophytic microbials

Juyong Park, Dong-Ku Kang^{1,*}

Department of Chemistry, INCHEON NATIONAL UNIVERSITY, Korea

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

This study aims to identify and develop antimicrobial substances that suitable for human body. Ninety six natural biological extracts were obtained from the culture broth of endophytic microbial. endophytic microbials were supplied from Korea Plant Resources Research Institute (KNIBR). Culture broths of endophytic microbial were extracted by liquid-liquid extraction in ethyl acetate and then concentrated samples were validated to identify antimicrobial activities using paper disk assay on sepsis-related pathogens including *Escherichia coli* (gram negative), *Staphylococcus aureus* (gram positive), *Klebsiella pneumonia* (gram negative), *Enterococcus faecalis* (gram positive), *Streptococcus pseudopneumoniae* (gram negative) and *Candida albicans* (yeast). Then, several whole extracts were validated that have excellent antimicrobial activities and here we focused on C10 sample to identify functional chemical compound within whole extract through fractionation using HPLC. Here we optimized fractionation condition to distinguish various chemical compounds within the whole extract and all fractions were tested to validate the antimicrobial activity using paper disc assay. Alama blue-based bacterial cell viability assay was also performed to verify IC₅₀ values from active fractioins and their structure was characterized using by NMR and mass spectrometry.

Poster Presentation : **MEDIP-435**

Medicinal Chemistry

Exhibition Hall 2, THU 11:00~12:30

Antibacterial activity and mechanism of action of chelation free Zn (II)azole complexes in Methicillin resistant Staphylococcus aureus

Sondavid Nandanwar

Department of Marine Convergence Design, Pukyong National University, Korea

In this study, we synthesized three chelation-free Zn (II) complexes $[ZnCl_2 L_2]$ of monodentate ligands with L= 2-isopropylimidazole (**L1**), 2-methylbenzimidazole (**L2**), and 2-methylbenzoxazole (**L3**) and evaluated their antibacterial activity. The chelation free properties of these organometallic complexes were characterized by UV-Vis spectroscopy, 1H -NMR spectroscopy, and single X-ray crystallography. Complexes **1-3** exhibited antibacterial activity against all antibiotic susceptible bacteria within the range of 100-200 $\mu g/ml$ while free ligands **L1** and **L2** exhibited antibacterial activity above 200 $\mu g/ml$. Both complexes **2** and **3** were twice more active against MRSA than complex **1**. SYTOX green uptake and DNA binding assay revealed that complexes **1-3** may kill bacterial cells by inhibition of translation and/or transcription upon cell permeabilization. Further, investigation is going on to find the exact mechanism of action of complexes **1-3**. Interestingly, complexes **2** had potent antioxidant activity than complex **1**, **3** and standard antioxidant rutin. Taken together, our results suggest that complexes **1-3** can be developed as novel antimicrobial and antioxidant agents.

Poster Presentation : **MAT.P-391**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Bi_xPd_y Alloy Particles Characterized by Catalytic Activity at Low Temperature: Nitro Reduction and C-C Coupling Reactions under Green Conditions

Kang Yeol Lee^{*}, Seung Heon Lee¹, Myong Yong Choi¹, Jineun Kim¹

Research Institute of Natural Science, Gyeongsang National University, Korea

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

A simple method for synthesizing the Bi_xPd_y alloy particles is described. The structure, composition distribution and size of synthesized Bi_xPd_y alloy particles were characterized using a number of analytical techniques. The Bi:Pd atomic ratio (x:y) of the particles was determined to be approximately 1:3 (Bi₂₄Pd₇₆), 1:1 (Bi₅₄Pd₄₆) and 3:1 (Bi₇₄Pd₂₆). The crystalline properties of the surface of the Bi_xPd_y alloy particles were observed in high-resolution transmission electron microscopy analysis. The d-spacings between the adjacent lattice planes were measured on the surface of Bi_xPd_y alloy particles by averaging 10 lattice fringes distance. The catalytic activity of Bi_xPd_y alloy nanoparticles was determined for the nitro compound reduction and C-C coupling reactions under green conditions (in water solution). Bi₁Pd₃ particles were shown to provide the best catalytic performance during both reactions, resulting in a yield of 98% in both cases.

Poster Presentation : **MAT.P-392**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Improved Photocurrent Extraction from PbS Quantum Dot Photovoltaics by Incorporation of Fullerene-Encapsulated Single-walled Carbon Nanotubes

Jonghee Yang, Junyoung Lee, Whikun Yi*

Department of Chemistry, Hanyang University, Korea

Single-walled carbon nanotubes (SWNTs) and C₆₀-encapsulated SWNTs (C₆₀@SWNT), are incorporated with a 1,2-ethanedithiol (EDT) treated PbS QD layer, which plays a role of hole extraction layer in PbS quantum dot photovoltaics (QDPVs). QDPVs incorporating SWNT (or C₆₀@SWNT) demonstrate significantly improved performance. photoinduced charge extraction by linearly increasing voltage (photo-CELIV) measurement, demonstrates that the incorporation of SWNT species provides efficient hole transport through the EDT-PbS film and suppresses the bimolecular recombination in the film, resulting in enhanced hole diffusion length. Considering depletion width and diffusion length of hole, the required transport length for hole extraction from QDPV is fully covered by incorporating C₆₀@SWNT with EDT-PbS QD, indicating photocurrent extraction from QDPV is significantly improved.

Poster Presentation : **MAT.P-393**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication and Applications of Noble Metal Coated Fe₃O₄@TiO₂ Photocatalyst Nanoparticles with Enhanced Activity

Kyeong-Mi Song, Seong-Hyun Jang, 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. TiO₂ 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 Fe₃O₄ 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 or Ag,Au-coated Fe₃O₄@TiO₂ particles with a good core-shell structure is demonstrated. As characterized by FE-SEM and XRD the as-synthesized Ag or Ag,Au-coated Fe₃O₄@TiO₂ nanoparticles exhibit a narrow size distribution. The Ag or Ag,Au-coated Fe₃O₄@TiO₂ photocatalyst exhibited high photocatalytic activity in the degradation of Rhodamine B (Rh.B) and Methyl orange (MO) under solar light and vis light. Finally, the photodynamic process of Ag or Ag,Au-coated Fe₃O₄@TiO₂ 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 ($\bullet\text{O}_2^-$), hydrogen peroxide (H₂O₂), singlet oxygen ($^1\text{O}_2$), and hydroxyl radical ($\bullet\text{OH}$) in photocatalysis, were comprehensively surveyed. Reactive oxygen species (ROS) confirmed once more under presence of the scavengers.

Poster Presentation : **MAT.P-394**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Heterolayered Organic Intercalation Compounds of Mixed Metal Oxide-Chalcogenide Nanosheets with Improved Electrocatalyst Performance

Yuseon Kim, Xiaoyan Jin, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Highly efficient electrocatalysts for hydrogen evolution reaction (HER) are synthesized by the intercalative hybridization of organic cation with mixed transition metal oxide (TMO)- transition metal dichalcogenide (TMD) host lattice achieved by the simultaneous restacking of these host nanosheets with organic cations. The obtained organic intercalation compounds with TMO-TMD nanosheets shows much higher HER electrocatalytic activity than do the pristine nanosheets. The positive effect of hybridization with exfoliated TMO nanosheet on the HER activity of TMD is attributable to the enhanced charge transfer kinetics and the provision of more active sites of TMD via the prevention of the self-stacking of TMD nanosheets. The present result clearly demonstrates that the application of mixed host lattice can provide a powerful way of exploring highly efficient electrocatalyst materials.

Poster Presentation : **MAT.P-395**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Layered Metal Carbide Nanosheet as an Efficient Additive for Exploring High Performance Hybrid Electrode for Supercapacitor

Xiaoyan Jin, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Efficient supercapacitor electrode materials of mesoporous metal oxide-metal carbide nanocomposites can be synthesized by incorporating small amount of exfoliated MXene (i.e. Ti_3C_2) nanosheets into restacked metal oxide nanosheets. The common negative surface charges of the exfoliated MnO_2 and Ti_3C_2 nanosheets make possible the formation of stable colloidal mixture of both the nanosheets. The addition of proton into this anionic colloidal mixture yields self-assembled MnO_2 - Ti_3C_2 nanocomposites. The obtained MnO_2 - Ti_3C_2 nanocomposites show much better electrode performance for supercapacitor than does the restacked MnO_2 nanosheet, underscoring the beneficial effect of Ti_3C_2 addition on the electrochemical activity of metal oxide nanosheet. The improvement of electrode performance upon the incorporation of Ti_3C_2 nanosheet is attributable to the enhancement of charge transfer property, as evidenced by electrochemical impedance spectroscopy. The present work clearly demonstrates the useful role of exfoliated MXene nanosheet as a conductive additive for exploring efficient metal oxide nanosheet-based hybrid electrode materials.

Poster Presentation : **MAT.P-396**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Beneficial Effect of Amorphous Structure on the Electrochemical Functionalities of Metal Oxide

Min Ji Kim, Xiaoyan Jin, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The effect of the amorphous structure of metal oxide on its electrochemical functionalities is investigated with amorphous MoO₂ and well-crystallized MoO₂. Amorphous MoO₂ nanoparticles are synthesized by soft-chemical redox reactions using KBH₄ at room temperature. The amorphous MoO₂ nanoparticles show better electrocatalytic hydrogen evolution reaction (HER) activity and sodium-ion battery (NIB) performance than does the well-crystallized MoO₂ material, which is attributable to the greater surface area, higher electrochemical stability and better charge transfer kinetics of the amorphous MoO₂ material. The present study highlights the beneficial effect of amorphous nature for optimizing the electrocatalyst/electrode performance of metal oxide.

Poster Presentation : **MAT.P-397**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Mesoporously Restacked Nanocomposites of Layered Double Hydroxide-Metal Oxide Nanosheets with Improved Catalyst Performance

Saeyoung Kim, Xiaoyan Jin, Seong-Ju Hwang*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Mesoporously restacked nanocomposites of layered double hydroxide (LDH)-transition metal oxide (TMO) are synthesized by electrostatically-driven self-assembly of cationic exfoliated LDH nanosheets and anionic exfoliated TMO nanosheets. The obtained LDH-TMO nanocomposites show outstanding electrocatalytic activities for oxygen evolution and oxygen reduction. Of noteworthy is that the hybridization of LDH with TMO is quite effective in improving its chemical stability. The beneficial effect of TMO incorporation on the electrocatalyst performance is ascribable to the increase of electrical conductivity and the provision of more surface active sites of LDH material. The present study clearly demonstrates that the incorporation of TMO nanosheets can provide a facile and efficient method to explore high performance bifunctional electrocatalyst materials as well as efficient catalysts for Li-O₂ batteries.

Poster Presentation : **MAT.P-398**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

White light-emitting colloids and films containing organic sensitizer/LRH:RE nanosheets

Hong-Gu Jeon, Song-ho Byeon *

Department of Applied Chemistry, Kyung Hee University, Korea

White light-emitting hybrid colloids and composite films based on efficient energy-transfer between Tb³⁺ and Eu³⁺ and organic sensitizer in the layered rare-earth hydroxides (LRHs) were successfully designed and assembled. Considering that flexible luminescent materials have attracted an extensive interest due to their applicability in optoelectronic devices, novel transparent white-emitting nano-composite films have been fabricated by using biocompatible polyvinyl alcohol (PVA). Salicylate (sal) was selected as an organic sensitizer to harvest UV-light. Eu³⁺-doped layered terbium hydroxide (LTbH:Eu), Tb³⁺-doped layered yttrium hydroxide (LYH:Tb), and layered yttrium hydroxide (LYH) were selected as host matrices for red, green, and blue light emitting hybrid materials, respectively. White light emission was readily achieved by simple mixing of resulting sal-LTbH:Eu, sal-LYH:Tb, and sal-LYH colloids with appropriate ratios. Highly increased photostability of salicylate in the interlayer space of LRH provides both colloids and composite films high performance durable for long period under UV irradiation.

Poster Presentation : **MAT.P-399**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Ceria/polymer composite films for UV screen

WooJu Jeon, Hong-Gu Jeon, Song-ho Byeon *

Department of Applied Chemistry, Kyung Hee University, Korea

Ceria has attracted extensive research attention due to its potential applications in a variety of research fields such as three-way automotive catalysts, solid oxide fuel cells, and optical and biomedical materials. In addition, ceria presents unique capabilities in the absorption of UV light. As UV-screen is needed as part of safe-sun practices to reduce the effects of carcinogenic and photodamaging solar UV radiation, there has been increasing research interest in employing ceria in anti-UV coating materials. However, constructing composite coating films using ceria and inorganic/polymer species with accurate control in the coating structure has remained a challenge. In this work, CeO_{2-x} nanoparticles smaller than 10 nm in diameter showing variable band gap energy were prepared for UV-blocking composite films. Considering a large amount of surface hydroxyl groups, CeO_{2-x} particles were dispersed in polyvinyl alcohol (PVA), a representative polymer matrix. Resulting Ceria/PVA composite films showed excellent UV-blocking performance.

Poster Presentation : **MAT.P-400**

Material Chemistry

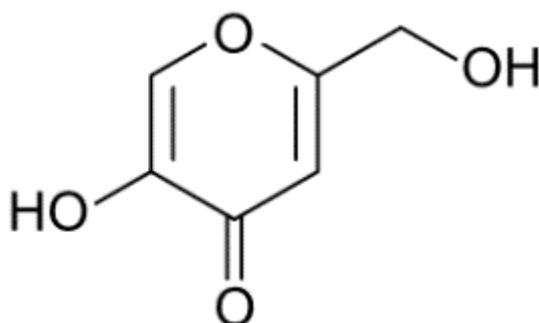
Exhibition Hall 2, FRI 11:00~12:30

Kojic acid intercalated layered yttrium hydroxide

Bora Kang, Song-ho Byeon *

Department of Applied Chemistry, Kyung Hee University, Korea

Despite their presence in small quantities in foods and plants, bioactive molecules provide great health benefits. However, because of high sensitivity to a number of factors such as light, temperature, and oxygen, it is important to stabilize these molecules and to find ways in preventing them from degradation to maximize their efficiency. Kojic acid as one of bioactive molecules, known to inhibit the formation of pigment in plant and animal tissues, is used on cut fruits to prevent oxidative browning, in seafood to preserve pink and red colors, and in cosmetics to lighten skin. It has also antibacterial and antifungal properties. In the present work, the layered yttrium hydroxide (LYH) was explored as a host material for the encapsulation of kojic acid to enhance its thermal and photo stabilities. The inclusion phenomena of kojic acid molecules into the interlayer gallery of LYH were compared with those into the interlayer of layered double hydroxide (LDH).



Poster Presentation : **MAT.P-401**

Material Chemistry

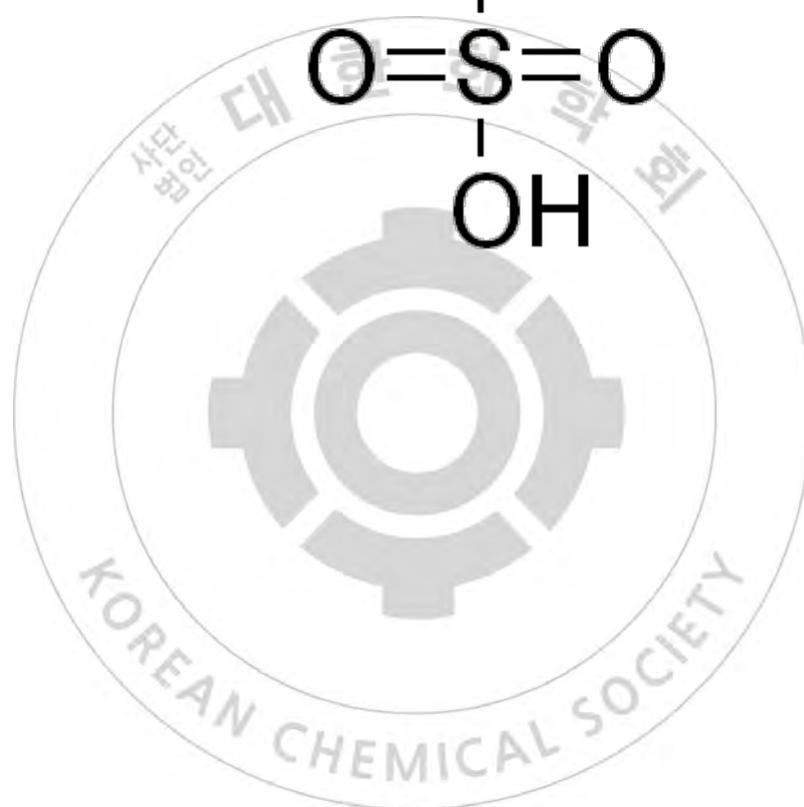
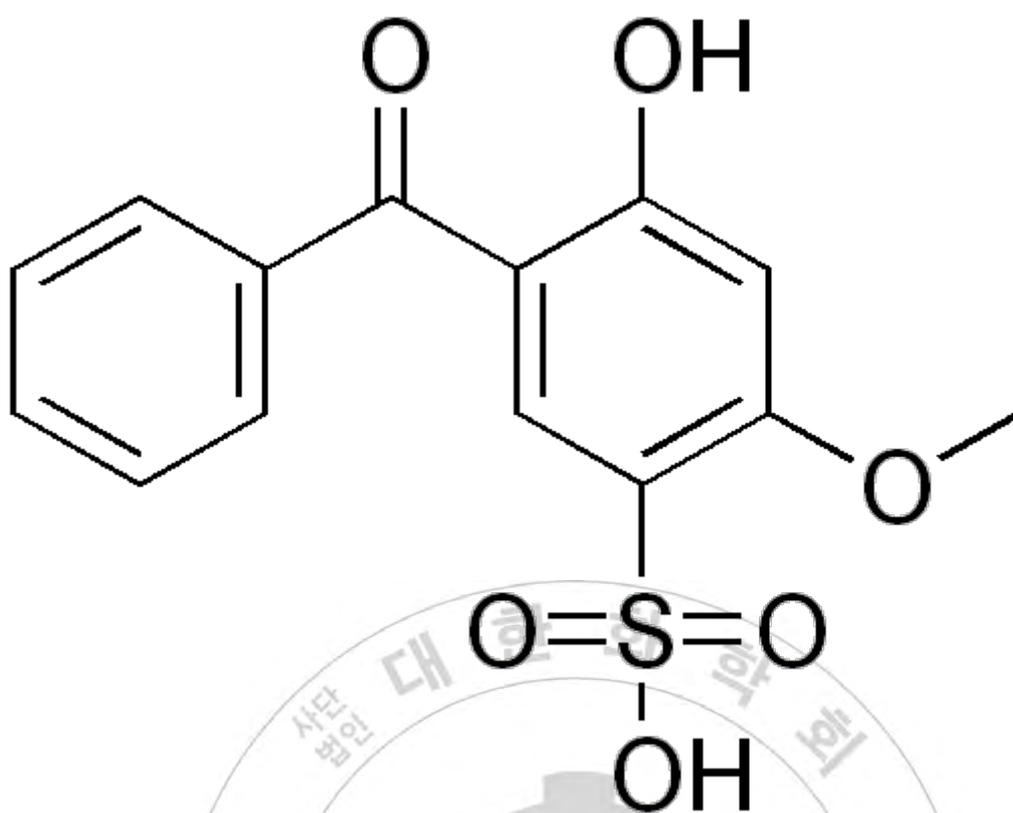
Exhibition Hall 2, FRI 11:00~12:30

Encapsulation of BP-4 sunscreens agent into LYH matrix to enhance its photostability

Juyeong Choi, Bora Kang, Song-ho Byeon *

Department of Applied Chemistry, Kyung Hee University, Korea

2-hydroxy-4-methoxybenzophenone-5-sulfonic acid (Benzophenone-4; BP-4) is commercially used for sunscreen protecting the skin from damage by a majority of UV radiation from the sunlight. However, BP-4 has been found to induce cosmetic dermatitis of the face and neck and also causes sensitization at other locations. Layered host matrices comprising inorganic ions interchangeable with organic ions are particularly of interest because guest organic molecules can be readily stored by an exchange reaction, protected in the interlayer space from aging by heat, UV light, and oxygen. Furthermore, a direct contact of organic guests with skin can also be avoided in the interlayer space. In the present work, BP-4 was encapsulated by the exchange reaction with the calcined layered yttrium hydroxide (c-LYH) because its direct intercalation into the interlayer space of LYH was unsuccessful. When confined in the interlayer space, the confinement effect resulted in a significant broadening and a shift to the longer wavelength region of the absorption bands of BP-4. In contrast to a significant decrease in UV-screening ability of free BP-4, an effective UV absorption performance of BP-4-LYH hybrid was maintained even after exposed to the simulated sunlight for 72 h.



Poster Presentation : **MAT.P-402**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of porous magnetic absorbents for oil/water separation

Yoseph Lee, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

With the increase in production of oily wastewaters and the strict regulations on its discharge, the development of materials and methods for oil/water separation is very critical to modern society. There are various types of oil/water separation environments. Among them, tricky situations that restrict man access have hindered efficient oil/water separation processes. Selective absorption of water or oil by hydrophilic or hydrophobic absorbent, respectively, is useful for industrial processes that use two, more, or mixed solvents. Moreover, hydrophilic or hydrophobic absorbent with a magnetic property has advantages over general absorbents if it is used in appropriate application fields. Herein, we report that hydrophilic or hydrophobic porous magnetic absorbents that possess enough magnetic force to be manipulated by an external magnetic field for tricky oil/water separation.

Poster Presentation : **MAT.P-403**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Amphiprotic air filters for removal of particulate matters (PM2.5)

Sol Park, Won san Choi^{1,*}

Chemical&Biological Engineering, Hanbat National University, Korea

¹*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-404**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Alginate-based macroscopic adsorbents for efficient removal of heavy metal ions

Han bi Lee, Won san Choi^{1,*}

Chemical & biological Engineering, Hanbat National University, Korea

¹*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

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

Exhibition Hall 2, FRI 11:00~12:30

N-doped carbon blacks by two step heating as a metal free catalysts for oxygen reduction reaction.

Sunhee Park, Sungjin Park*, Yunseok Shin

Department of Chemistry, Inha University, Korea

Two step heated carbon black is a excellent electrochemical oxygen reduction reactions (ORRs) catalysts, in terms of efficient, durable, and cost-effective catalysts. In this regard, the development of metal-free catalysts with excellent activity is essential. Herein we report the development of a novel two-step heating route to produce metal-free N-doped carbon blacks. The prepared materials exhibit superior electrocatalytic performance for ORRs in a basic media, which is comparable to commercial Pt/C catalysts. Among the various heating temperatures tested, sequential two-step heating at 750 and 1000 °C produced the most efficient catalysts with onset and half-wave potentials of 0.97 and 0.82 V, respectively. The prepared materials show excellent selectivity for 4-electron transfer, durability, and stability in response to methanol poisoning. Control experiments with one-step heating and no N-doping confirm the superiority of the two-step heating process for producing efficient electrocatalysts.

Poster Presentation : **MAT.P-406**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Order for Production Steps on N-doped Reduced Graphene Oxide/Fe₃O₄ Hybrids on Electrocatalytic Performances for Oxygen Reduction Reaction

Dawoon Jang, Sungjin Park*

Department of Chemistry, Inha University, Korea

Graphene-based materials are promising as transition metal, cost-effective electrocatalysts owing to their feasibility for mass production and excellent electrochemical properties. Recently, Fe, Co doping of graphene networks has been identified as a promising route to produce efficient electrocatalysts for the oxygen reduction reaction (ORR). Oxygen reduction reactions (ORRs) occur at cathodes in fuel cells and require efficient electrocatalysts. Because of the cost and limited durability and stability of commercial Pt/C catalysts, the development of efficient Pt-free electrocatalysts is an active research topic. Here, we describe the solution-based production of Fe₃O₄ nanoparticles/N-doped graphene-based materials from FeCl₂, graphene oxide(G-O), and hydrazine. Orders of production steps were varied by; i) reacting FeCl₂ and G-O first and then adding hydrazine (Fe/G-N), ii) reacting G-O, FeCl₂, and hydrazine at the same time (Fe/G/N), or iii) reacting G-O and hydrazine first and then adding FeCl₂ (G/N-Fe). The hybrids produced showed better ORR electrocatalytic activity in alkaline media than single components such as N-doped graphene-based materials or Fe₃O₄. Furthermore, the electrocatalytic properties of the resulting hybrids were found to depend on orders of addition. Fe/G/N was found to be the best electrocatalyst and had better onset and half-wave potentials, thermodynamic current density, and 4-electron selectivity. All three hybrids show good cyclic durability and methanol tolerance.

Poster Presentation : **MAT.P-407**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Uniformly-dispersed Pt nanoparticles on borane-modified graphene oxide as electrocatalyst for oxygen reduction reaction

Sujin Seok^{*}, Haeju Kim, Sungjin Park

Department of Chemistry, Inha University, Korea

The oxygen reduction reaction (ORR) at cathode is critical in the electrochemical energy conversion systems, such as fuel cells and metal-air batteries. ORR at the cathode during redox reactions is sluggish reaction so then requires effective electrocatalysts to overcome the high activation energy. Pt/C catalysts have been known the best catalytic activity because of the superior catalytic ability of Pt particles. However, it is still a challenge to synthesis efficient ORR catalysts containing Pt species by solution processes at low temperatures. In this work, we report a new route for producing hybrids ORR catalyst consist of well-dispersed Pt nanoparticles of uniform size on the surface of borane-reduced graphene oxide (BG) using a low-temperature solution process. The Pt particles have 10–15 nm size-distribution and are well-dispersed on the surface of BG without agglomeration. The Pt-BG hybrid catalysts exhibit excellent electrocatalytic activity with high onset and half-wave potentials of 0.99 and 0.84V respectively. When compared with Pt/C and previously reported Pt-based catalysts, the hybrids are comparable to those catalyst and also show excellent four-electron selectivity and superior kinetics.

Poster Presentation : **MAT.P-408**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Size-Dependent Nonthermalized Energy Transfer in Dye-Conjugated Gold Nanoclusters

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department of chemistry, Yonsei University, Korea

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Energy transfer is one of the most important properties that enables the luminescence-based techniques to be used in large areas. Above all, nonthermalized energy transfer is a unique property that occurs in donor's long-lived upper excited state. This is usually shown at specific molecules like carotenoids. Recently, nanoclusters have suggested as alternative of quantum dots in energy transfer region because of their stability, low toxicity, etc. In this work, we observed nonthermalized energy transfer in dye-conjugated gold nanoclusters. 6-aminofluorescein(AF) was conjugated to various size of glutathione(SG) protected gold nanoclusters by using dicyclohexylcarbodiimide(DCC). As nanoclusters are not soluble in organic solvent, least amount of water was mixed to main solvent, acetone. The activity of DCC is inhibited by water, but this means that the binding number of AF can be controlled. Comparing nanoclusters of different sizes with the same AF conjugation numbers, Au₁₈-AF shows much brighter emission while Au₁₀₂-AF shows similar emission with SG-AF even it has much intense absorption near 490nm. This phenomenon cannot be explained by FRET theory including spectral overlap concept. To finding the origin of size-dependent emission, transient absorption measurement was proceeded. It confirms that nonthermalized energy transfer occurs only in small-sized nanoclusters, which is the same trend as PL results. It is well known that small-sized nanoclusters have slower relaxation rate compared with large nanoparticles. Based on principle of nonthermalized energy transfer, slower intracore relaxation may induce highly efficient energy transfer. This result shows the potential that nanoclusters can be a valuable platform for luminescence system.

Poster Presentation : **MAT.P-409**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Functionalization of graphene quantum dot for electrocatalysis and photocatalysis

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

Carbon based nanomaterials have attracted much attentions due to their special physicochemical properties and diversiform shapes. Graphene quantum dots (GQDs) are defined as graphene sheets with few to ten layers and lateral dimensions < 100 nm. Zero-dimensional (0D) GQDs exhibit outstanding optical activity, robust chemical inertness due to their quantum confinement and edge effects. In this regard, modification of GQDs has been emerged as efficient approach for achieving superior nanosensors for selective detection of chemical and biological molecules. In this study, we report a simple method to prepare surface-functionalized GQDs by organic sulfur compounds, which exhibited enhanced electrocatalytic and photocatalytic performances. The relationships between the photocatalyst structure and the photocatalytic activities are discussed in detail.

Poster Presentation : **MAT.P-410**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of polyaniline-loaded metal-organic framework MIL-101(Cr) for CO₂ capture with increased capacity and selectivity

Dongkyu Yoo, Sung Hwa Jhung*

Department of Chemistry, Kyungpook National University, Korea

Highly porous metal-organic framework (MOF), MIL-101(Cr), was modified by introduction of polyaniline (PANI) via ship in bottle strategy in order to utilize basic moieties of PANI in capturing CO₂ effectively from flue gas. PANI@MIL-101(Cr), with suitable PANI concentration, showed highly increased adsorption capacity for CO₂, especially at low pressure of 0.15 atm, even though the porosity of MIL-101(Cr) was decreased upon PANI loading. Moreover, the PANI@MIL-101(Cr) showed increased selectivity for CO₂ (against N₂), compared with pristine MIL-101(Cr); and stable reusability. The observed favorable adsorption of CO₂ on the PANI@MIL-101(Cr) might be because of basic species on well-dispersed PANI on the MOF. The results indicate that modification of porous materials such as MOFs with PANI might be one way to improve performances for CO₂ capture

Poster Presentation : **MAT.P-411**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Bimetallic-MOF-74s derived porous carbons with well-dispersed Ni-/MnO-nanoparticles for highly reactive redox catalysts

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Kyungpook National University, Korea

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

A series of bimetallic metal-organic framework-74s (MOF-74s) (Zn/Ni or Zn/Mn in various compositions), were synthesized, and Ni or MnO-doped carbonaceous materials were firstly prepared by direct carbonization of the MOF-74s under an inert environment for applying in redox catalysis. The obtained MOF-derived nanomaterials (MDNMs) were characterized thoroughly to understand their physicochemical properties including phase, porosity, particle size, dispersion, and composition. The porosity of the MDNMs increased but the size and content of Ni or MnO in the MDNMs decreased monotonously with increasing Zn content in the bimetallic MOF-74s. One MDNM(75Zn25Mn), prepared from MOF-74(75%Zn/25%Mn), showed noticeably higher activity in the oxidation of benzyl alcohol as compared with not only the MDNM(xZnyMn)s but also MnO_x-loaded carbon or loaded γ -alumina (or, MDNM(75Zn25Mn) showed ~ 54 times turnover frequency (TOF) to that of MnO/activated carbon). MDNM(75Zn25Mn) was also effective in the oxidative removal of dibenzothiophene from a model fuel. Moreover, MDNM(75Zn25Ni), prepared from MOF-74(75%Zn25%Ni), had the highest TOF in the reduction of 4-nitrophenol among various MDNM(xZnyNi)s. The highest activity of MDNM(75Zn25Mn) and MDNM(75Zn25Ni), even with the lowest Mn and Ni contents in the respective MDNMs, for oxidation and reduction in several cycles might be due to the well-dispersed MnO (and Ni) and high porosity with mesopores. Therefore, it can be suggested that pyrolysis of MOFs composed of mixed-metal can be a facile way to get highly effective and reusable heterogeneous catalysts, with small sized and uniformly-dispersed active species, for various organic redox reactions.

Poster Presentation : **MAT.P-412**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Adsorption removal of benzothiophene from liquid fuel with ionic liquid supported metalorganic framework

JongMin Park, Sung Hwa Jung*

Department of Chemistry, Kyungpook National University, Korea

Sulfur containing compounds in liquid fuels are considered as the sources of the toxic SO_x emission. Therefore, there is a considerable demand to reduce those compounds from marketable fuels 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-413**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Efficient photocatalytic degradation of methylene blue by RuO₂-CNT nanocomposite

Jidang Kim, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

Photodegradation of organic pollutants by oxide-based photocatalysts has gained increasing attention as a solution to environmental problems. Generally, the degradation of pollutants proceeds by reaction with reactive hydroxyl radicals, which are generated by the reaction of water molecules adsorbed onto the photocatalyst with photogenerated charge carriers in the photocatalyst. However, the fast recombination rate of photogenerated charge carriers limits the ability for enhanced catalytic efficiency of oxide based photocatalysts. The difficulty of separating and recycling these catalysts also hinders their practical application. In this study, we report on the preparation and photocatalytic properties of a RuO₂-carbon nanotube (RuO₂-CNT) nanocomposite, comprised of RuO₂ nanoparticles deposited onto a thiolated CNT substrate by wet chemical methods. The RuO₂-CNT nanocomposite was characterized by spectroscopic methods. The photocatalytic activity of the RuO₂-CNT nanocomposite was evaluated using degradation of methylene blue (MB) under UV-vis light.

Poster Presentation : **MAT.P-414**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Non-enzymatic amperometric determination of hydrogen peroxide using ZnO-CNT

Jidang Kim, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

Hydrogen peroxide (H_2O_2) is widely used as an antibacterial, bleaching, decoloring, and oxidizing agent in various industrial fields. However, the exposure to and accumulation of high levels of H_2O_2 can cause oxidative stress to humans, leading to caducity and diseases due to its unstable and toxic nature. Moreover, H_2O_2 is a useful indicator for monitoring reactive oxygen species-related diseases in humans because it is generated as an intermediate product of many enzymatic reactions in normal aerobic metabolism. It is therefore essential to develop accurate and reliable methods of detecting H_2O_2 for industrial and biological purposes. In this study, ZnO-CNTs were prepared by a sol-gel method and their potential application for non-enzymatic amperometric detection of H_2O_2 was examined. The modified electrode exhibited good sensitivity and detection range for H_2O_2 sensing. The enhanced sensing performances can be attributed to the superior electron transport and the large effective surface area resulting from the smaller size and excellent dispersion of ZnO nanoparticles on the CNT.

Poster Presentation : **MAT.P-415**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Phase-Selective Synthesis of Two-Dimensional MoTe₂ through Te Flux Control

Hyeonkyeong Kim, Youngdong Yoo^{1,*}

Department of Energy Systems Research, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

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-416**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

An effective Storage Materials of Sodium Ion battery using a Covalent Organic Nanosheets(CONs).

Kim Min-Sung, Jin Kuen Park*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

We conducted six types of covalent organic nanosheets(CONs) under two different conditions, reflux and solvothermal reactions, using a Stille cross-coupling for energy storage. Surface area and self-assembled morphology of the CONs could be adjusted according to the monomer selection and synthesis method. Sodium-ion storage capacity in the mentioned above CONs could be increased by elevating their conductivity of charge carriers via enforcement of a network polymer backbone planarity or by enhancing their specific surface area while maintaining polymer structure constitution. Comparing the anodes manufactured by combining each synthesized CONs, the electrodes based on CON-16 showed the highest cycling performance and rate capability, maintained a reversible discharge capacity of up to 250mAh/g after 30 cycles at a current density of 100 mA/g. and showed the highest cycling performance and rate capability.

Poster Presentation : **MAT.P-417**

Material Chemistry

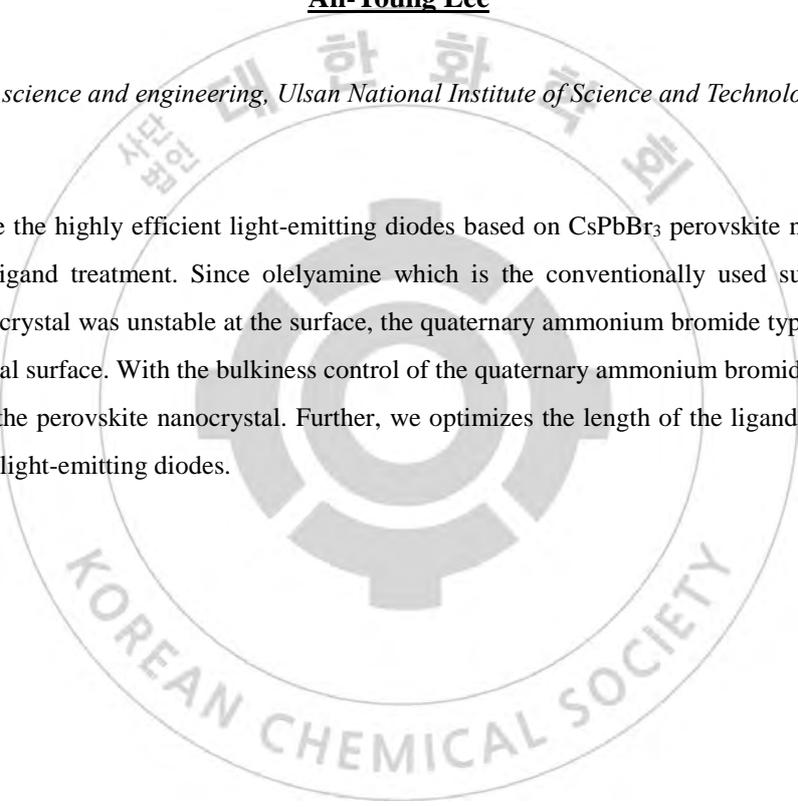
Exhibition Hall 2, FRI 11:00~12:30

Perovskite nanocrystal based highly efficient light-emitting diodes with post-synthetic ligand treatment

Ah-Young Lee

Materials science and engineering, Ulsan National Institute of Science and Technology, Korea

We demonstrate the highly efficient light-emitting diodes based on CsPbBr₃ perovskite nanocrystal with post-synthetic ligand treatment. Since olelyamine which is the conventionally used surface ligand in perovskite nanocrystal was unstable at the surface, the quaternary ammonium bromide types were applied to the nanocrystal surface. With the bulkiness control of the quaternary ammonium bromide, we optimizes the stability of the perovskite nanocrystal. Further, we optimizes the length of the ligands to achieve the highly efficient light-emitting diodes.



Poster Presentation : **MAT.P-418**

Material Chemistry

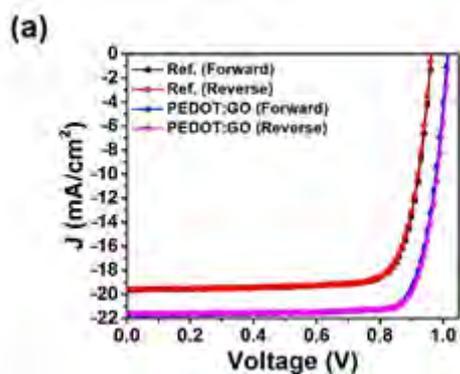
Exhibition Hall 2, FRI 11:00~12:30

Enhancing performance of perovskite solar cells introducing PEDOT:PSS and GO composite layer as a hole transport layer

Ji A Hong

Ulsan National Institute of Science and Technology, Korea

we studied efficient and stable perovskite solar cells (PSCs) using PEDOT:PSS:graphene oxide(GO) composite layer as a hole transport layer. The enhanced performance of device with PEDOT:GO composite layer comes from good optical and electrical properties of the PEDOT:GO layer. Benzoid-quinoid transition of PEDOT:PSS and higher work function of PEDOT:PSS and GO composite layer enhances charge transport ability. Moreover, improved morphology of the perovskite layer suppresses leakage current. The device with the PEDOT:PSS and GO composite layer shows superior long-term stability in ambient air. The maximum value of PSCs shows power conversion efficiency of 18.09% which is higher value compared to the solar cell with PEDOT:PSS layer.



Poster Presentation : **MAT.P-419**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photocatalytic degradation of rhodamine B dyes by TiO₂ and Au nanoparticles supported on the PDMS sponge under UV and visible light irradiation

Seong Youl Lee, Joon Heon Kim*

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

A porous PDMS (polydimethylsiloxane) sponge was simply fabricated by sugar cube templating method based on capillary suction of pre-PDMS polymer into sugar cubes. Then, TiO₂ nanoparticles (NPs) and AuNPs were successfully deposited inside and outside of PDMS pores by physical adsorption and chemical reduction processes, respectively. Importantly, our simple method is an environment-friendly synthesis without the requirement of additional reducing, stabilizing and functionalizing agents. Characteristics of the PDMS-TiO₂-Au sponge were evaluated by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and UV-vis spectroscopy. The size of macropores varies from 91 to 900 μm and the TiO₂ NPs predominantly exist in aggregate states, and the AuNPs with a size of 18-45 nm are formed. Photocatalytic activity was monitored by decoloration of rhodamine B solution under UV and visible light irradiation. The PDMS-TiO₂-Au sponge shows higher photocatalytic activity than that of pristine TiO₂ particles or AuNPs due to synergistic effects of adsorption, photocatalytic reaction and surface plasmon resonance.

Poster Presentation : **MAT.P-420**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Interdigitated electrodes pattern for liquid dielectrophoresis paper chip.

Sooyong Park, Veasna Soum, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

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 of droplet. 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 electric field is applied in the opposite direction of the droplet is uniform, the magnitudes of the electrostatic forces applied on particles are same, so the net force applied on the particles becomes zero and the particles do not move. However, If 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 move to part where the density of electric field is high due to the gradient of the electric field. Therefore, in the interdigitated electrodes, due to difference of electric field density, liquid dielectrophoresis occurs. Therefore, the use of liquid dielectrophoresis force can easily control the various motions of droplet underlying chemical reactions on paper based open DMF chips.

Poster Presentation : **MAT.P-421**

Material Chemistry

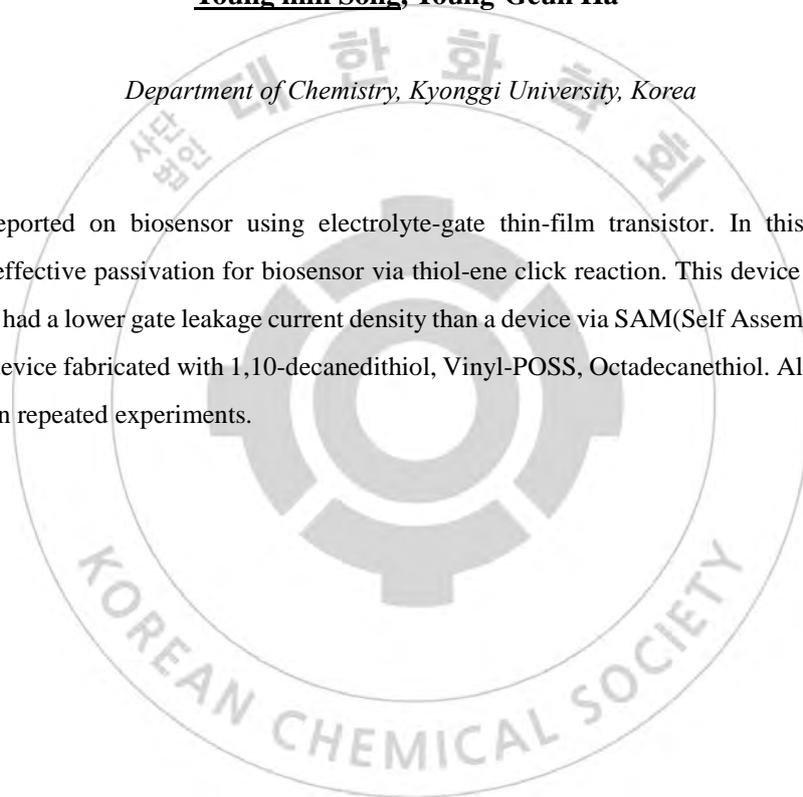
Exhibition Hall 2, FRI 11:00~12:30

Effective Passivation for Biosensor using Electrolyte-gate Thin-Film Transistor

Young min Song, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Recently, it reported on biosensor using electrolyte-gate thin-film transistor. In this study, we had demonstrated effective passivation for biosensor via thiol-ene click reaction. This device is fabricated via UV curing and had a lower gate leakage current density than a device via SAM(Self Assembled Monolayer) method. This device fabricated with 1,10-decanedithiol, Vinyl-POSS, Octadecanethiol. Also, these devices function well in repeated experiments.



Poster Presentation : **MAT.P-422**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Preparation of superhydrophobic film at room temperature by a facile UV process and Self-Assembled Monolayer Nanoparticles

Yeonah Park, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

In this experiment, we can get superhydrophobic film by simple spray coating process at room temperature (RT). We synthesized a material by thiol-ene click reaction between V-POSS and Octadecanethiol under UV radiation at RT. The vinyl functional groups were substituted with octadecanethiol. And to increase the roughness, we obtained self-assembled Al₂O₃ nanoparticles with Octadecyltriphosphonic acid (ODPA). After spray coating with the made materials, the film showed superhydrophobicity by substitution with octadecanethiol which has low surface energy and by increased roughness. The coated film results in a water contact angle greater than 150° and a small sliding angle (SA ≤ 10°). In addition, after sonication, partially, the coated surfaces still retained the superhydrophobicity.

Poster Presentation : **MAT.P-423**

Material Chemistry

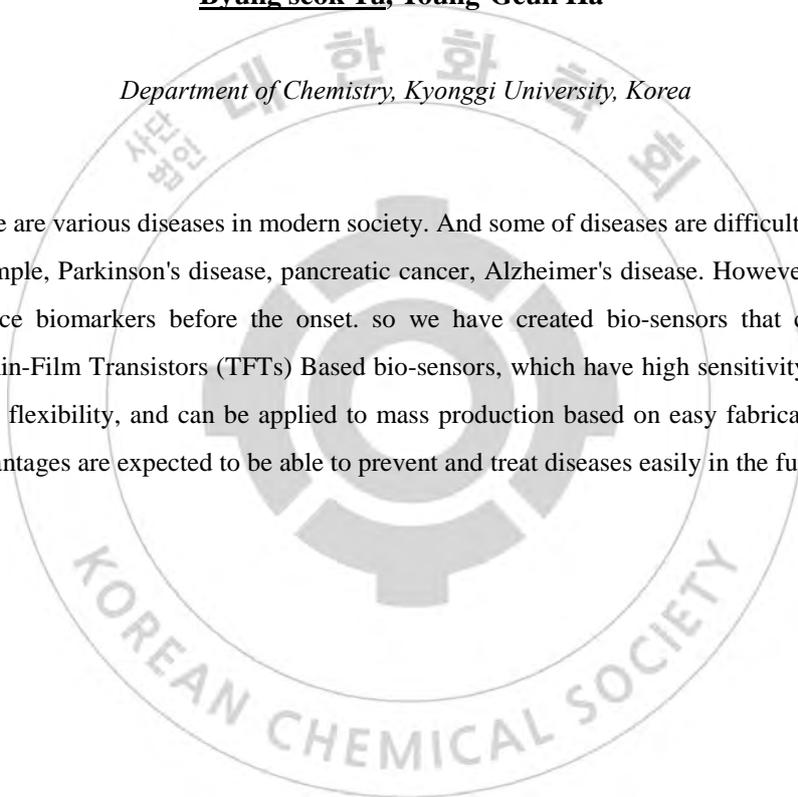
Exhibition Hall 2, FRI 11:00~12:30

Study on Thin-Film Transistor (TFT) Based Bio-sensor Application with bottom-gate top-contact structure

Byung seok Yu, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Recently, There are various diseases in modern society. And some of diseases are difficult to treat after the onset. For example, Parkinson's disease, pancreatic cancer, Alzheimer's disease. However, some of these diseases produce biomarkers before the onset. so we have created bio-sensors that can detect these biomarkers. Thin-Film Transistors (TFTs) Based bio-sensors, which have high sensitivity, low cost, easy fabrication and flexibility, and can be applied to mass production based on easy fabrication. Biosensors with these advantages are expected to be able to prevent and treat diseases easily in the future.



Poster Presentation : **MAT.P-424**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Stretchable batteries with gradient multilayer conductors

Minsu Gu, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

Stretchable conductors are essential components in next-generation deformable and wearable electronic devices. The ability of nanocomposite materials to achieve sufficient electrical conductivity, however, remains limited under high strain, which is particularly detrimental for charge storage devices. In this study, we present stretchable conductors made from multiple layers of gradient assemblies of polyurethane (GAP) comprising gold nanoparticles capable of self-assembly under strain. Stratified layering affords control over the composite internal architecture at multiple scales, leading to metallic conductivity in both the lateral and transversal directions under strains as high as 300%. The unique combination of the electrical and mechanical properties of GAP electrodes enables the development of a stretchable lithium-ion battery with a charge-discharge rate capability of 100 mAh g⁻¹ at a current density of 0.5 A g⁻¹ and remarkable cycle retention of 96% after 1,000 cycles. The materials engineering concept of hierarchical GAP nanocomposites can be generalized as a variety of nanoscale components, and the simplicity of their preparation affords rapid scale-up of fabrication of advanced charge storage devices.

Poster Presentation : **MAT.P-425**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Evaluating the electrical quality of powder-type graphene materials

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¹Department of Nano & Advanced Materials Engineerin, Jeonju University, Korea

A test method to evaluate the quality of powder-type graphene products such as reduced graphene oxide (rGO) and graphene nanopowder (GNP) was developed in this study. The pelletizer was selected for a sampling tool, which enables us to formulate the product as a measurable sample. Various parameters were measured from the pelletized sample in order to elucidate the best parameter for representing the quality of the graphene flakes in terms of their electrical properties. Based on the analysis of 4-probe measurement data on the pelletized sample, the best intrinsic parameter is volume resistivity (or volume conductivity) rather than resistivity (or conductivity). In addition, the possible modification of a sample before and after pressurization was investigated by electron microscopy and Raman spectroscopy. Any significant modification was not observed. The volume conductivity in the two types of the graphene was different from their individual conductivities by one order of magnitude. It was governed by the oxygen content included in the sample based on the results of X-ray photoelectron spectroscopy and Raman spectroscopy. Our achievements will promote the effective use of the powder-type graphene products for further applications.

Poster Presentation : **MAT.P-426**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Reusable Polybenzimidazole Nanofiber Air Filter for PM_{2.5} Dust Proof Mask

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Recently, ultrafine particulate matters (PMs) are serious causes of air pollution. The size of ultrafine PMs is similar or even smaller than that of human tissues, thus PMs are easy to accumulate in the body and may cause respiratory disease. Many researchers have developed a variety of dust-proof masks that filter out fine dust. However, in order to increase the dust-proof efficiency, most commercial filters are made of relatively thick and dense microfiller, resulting in a significant pressure drop, which can lead to uncomfortable breathing. In this work, we developed electrospun polybenzimidazole (PBI) nanofiber filters, and investigated its PM_{2.5} dust-proof filtering performance for potential use as dust-proof mask filters. The PBI has a high dipole moment (6.12 D) as confirmed by density function theory (DFT) calculations. The kelvin probe force microscope (KPFM) measurement confirms that the surface potential of the PBI nanofiber filter is higher than the surface potential of other commercial filters. The PBI air filter exhibits a high PM filtering efficiency (~ 98.5%) with much lower pressure drop (130 Pa) than commercial masks (pressure drop of 386 Pa) with similar filtering efficiency. We have also developed an effective cleaning method for filters contaminated with inorganic and organic PMs to reuse filters with negligible performance degradation. This research was supported by Creative Materials Discovery Program (NRF-2017M3D1A1039379) through the National Research Foundation of Korea(NRF) funded by Ministry of Science and ICT, and Korea Ministry of Environment (MOE) as “Advanced Technology Program for Environmental Industry Program”.

Poster Presentation : **MAT.P-427**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Ultrasonic Spray Chemistry: In-Situ Synthesis and Fabrication of Thin-Film Conjugated Microporous Polymer and Their Energy Storage Application

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Conjugated microporous polymers (CMPs) are potential materials for energy storage application owing to their rigid and cross-linked microporous structures. However, it is still a challenge to form film-like CMPs and integrate the CMPs into devices for further application because of its poor solubility and processability issues. Herein, we present a simple and very fast method to synthesize film-like CMPs by ultrasonic spray chemistry (USC), which allows in-situ polymerization and thin-film fabrication process simultaneously. By using USC, the oxidative coupling of triphenylamine (TPA) based monomers are easily achieved to produce the three different types of CMP-films that have different core units between TPA group, CMP-TPA, CMP-DTT, and CMP-BT. Compared with standard batch chemistry method of oxidative coupling reaction, USC delivers enhancement of synthetic yield of CMP-films because of releasing of enormous energy by collapsing of vacuum bubble that is formed during cavitation. As the increase of ultrasound frequency from 120 kHz to 180 kHz, the synthetic yield and porosity of CMP-films were also enhanced. We applied CMP-films to supercapacitor owing to their thin-film and microporosity. CMP-BT (180 kHz) exhibited much higher capacitance 250 F/g than 91 F/g for CMP-TPA (180 kHz), and 49 F/g for CMP-DTT (180 kHz) due to its polarized structures. Furthermore, layer-by-layer (LBL) CMP-BT (180 kHz)/single-wall carbon nanotube (SWCNT) electrode was prepared by USC for increasing conductivity and porosity of electrodes. This electrode demonstrated very high specific capacitances (583 F/g), and high cycling stability (95% retention after 20,000 cycles). This result suggested that USC offer a new way for overcoming the present processability issues of microporous materials.

Poster Presentation : **MAT.P-428**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Tuning the Luminescent Properties of Upconverting Nanoparticles via Multi-layer Structure

Dohyun Jeon, Young Sik Lee*, Doo-Hyun Ko*

Department of Applied Chemistry, Kyung Hee University, Korea

Upconverting Nanoparticles (UCNPs) follow the multi-photon optical process which involves the conversion of lower-energy photons into higher-energy photons. Generally, Rare-earth (RE) materials have been selected as dopant in the synthesis of UCNPs due to their unique converting capability; they possess the sharp and specific emission peak because of the ladder-like energy level. However, the conventional UCNPs, such as the core-shell structure consists of the single RE doped layer, could only emit the limited wavelength light. In this study, we synthesize NaYF₄:TmYb-NaYF₄:ErYb-NaYF₄, NaYF₄:ErYb-NaYF₄:TmYb-NaYF₄ core-shell-shell structures which show 'color tunable' optical property by regulating the induced light intensity. With these UCNPs, we not only controlled the emission wavelength without the other chemical treatment, but also applied to optical structure with maintain the photoluminescence character.

Poster Presentation : **MAT.P-429**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile synthesis of FA-doped CsPbBr₃ Perovskites Nanocrystals at Room temperature for Light-Emitting Diode (LED)

Jisun Lee, Jiyun Jung, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

Lead halide nanocrystals (NCs) perovskites CsPbBr₃ and FA-doped CsPbBr₃ (FA=Formamidinium)(CH(NH₂)₂) are synthesized at room temperature without the protection of inert gas for low-cost optoelectronics and photonics. The free amino groups are employed as surface ligands for growing perovskites NCs with a size of ~ 22nm. The PL emission peaks of pure and FA-doped CsPbBr₃ NCs shift from 514 to 518nm with increase amount of doped FA ion and the bandwidth of peaks is narrow (full width at half maximum (FWHM) of 26~28 nm). In addition, we demonstrate the electrical and electroluminescence performance of solution-processed light-emitting diodes (LEDs) based on our perovskites NCs. These results demonstrate that the as-obtained colloidal perovskites NCs are promising solution-processed emitter for LED in the future applications.

Poster Presentation : **MAT.P-430**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

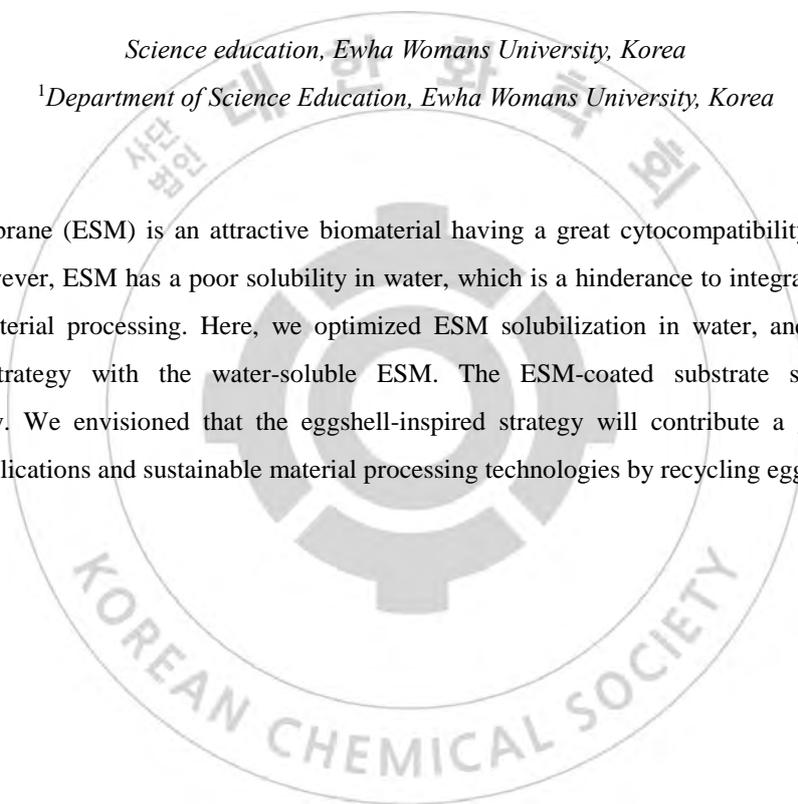
Eggshell-Inspired Strategy for Cytocompatible Nanocoating

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Eggshell membrane (ESM) is an attractive biomaterial having a great cytocompatibility and biological functions. However, ESM has a poor solubility in water, which is a hinderance to integrate ESM into the existing biomaterial processing. Here, we optimized ESM solubilization in water, and developed the nanocoating strategy with the water-soluble ESM. The ESM-coated substrate showed a great cytocompatibility. We envisioned that the eggshell-inspired strategy will contribute a great impact on biomedical applications and sustainable material processing technologies by recycling eggshells.



Poster Presentation : **MAT.P-431**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Carbazole Dioxazine-containing fused ring molecules displaying halochromic behavior in solution and film state

Youngun Kim, Jiwon Yoon¹, Chae Yeong Kim¹, Min Ju Cho, Dong Hoon Choi*

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¹*Chemistry, Korea University, Korea*

The halochromic effect was available to pigment based carbazole dioxazine (CzDxz) compound which embedded oxazine rings in the structure. Due to the poor solubility in organic solvents, CzDxz pigment was introduced and suggested with attachment of lengthy branched alkyl chains to the 9-position of each carbazole moiety, and moderate solubility in organic solvents including dichloromethane, chloroform, tetrahydrofuran was achieved. The effects of halochromism on the molecular structure, optical properties and the eventual sensor performance were investigated. Application of chromophore based on a fused nine-ring to the heteroaromatic system exhibited unexpected halochromism with significant shifts in λ_{\max} as large as 256 nm. The shift in the light absorption induced the phenomenon of original color turning blank, which is seen as transparent by NIR absorption under acid addition. Thin film optical properties of CzDxz were also found useful as pH sensor capable of fast interaction under acid condition. Sensor with immediate response and discrete optical change and transparency has potentially wide applications including industrial hazard sensors and those sensors attached to optoelectronics which utilize its transparency.

Poster Presentation : **MAT.P-432**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Aggregation Induced Emission Luminogens for Solution-processed Non-doped White Organic Light-emitting Diodes

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Kim, Su Hong Park, Min Ju Cho, Dong Hoon Choi***

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Recently, organic light emitting diodes (OLEDs) based on Aggregation Induced Emission (AIE) for the realization of non-doped OLEDs has been actively studied. Moreover, the device fabrication method of solution process was considered as a strategy for controlling the doping concentration with the desired composition which are advantageous for its simple, low cost, and large area display panel manufacturing. In this study, two dendritic luminogens of 3ICz-Tr and Tri-tNID were synthesized as blue and orange-red emitter, respectively, and also used for the application of white OLEDs (WOLEDs). Interestingly, the two luminogens showed unique AIE, which was measured by photoluminescence (PL) spectroscopy. As a non-doped emitting layer in the OLED devices, 3ICz-Tr and Tri-tNID showed maximum external quantum efficiency (EQEmax) of 7.29% and 3.71%, respectively. In addition, the WOLED device using 3ICz-Tr and Tri-tNID (99.5:0.5 wt. ratio) under host-free conditions demonstrated nearly pure white emission with the EQEmax of 8.32% and CIE coordinate of (0.32, 0.30).

Poster Presentation : **MAT.P-433**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solution-processed host-free WOLED fabricated with blue and red fluorescence blending film

**Chae Yeong Kim, Jiwon Yoon¹, Cheol Hun Jeong¹, Hyung Jong Kim¹, Youngun Kim¹,
Jihyun Kim, Min Ju Cho¹, Dong Hoon Choi^{1,*}**

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Recently, Non-doped white OLEDs have been attracting much attention due to the low-cost and easy fabrication process which offered offer great applications in display and lighting source. Doped emitting layer in conventional OLEDs have been reported in many literatures, but research on host-free systems is not much explored yet. In this study, star-shaped 3Py-DPAc and InDPAc-BT-CN were synthesized as blue emitter and red emitter, respectively, to realize non-doped white OLEDs. 3Py-DPAc showed good solubility and aggregation induced emission behavior which are favorable for non-doped solution-processed system. White OLED system has been driven by charge transfer and charge trapping mechanisms from blue to red emitter. Finally, 3Py-DPAc and InDPAc-BT-CN were blended to compose a single emitting layer in white OLED. As a non-doped system WOLED devices, it showed CIE coordinates of (0.32, 0.34) which is close to pure white.

Poster Presentation : **MAT.P-434**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Supramolecularly Controlled Second-Order Stark Effect in an Organic-molecular Diode

Soo jin Cho, Gyu Don Kong, Sohyun Park, Hyo Jae Yoon*

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Understanding the supramolecular structure-electric field relationship is a significant chemical challenge in various research areas. We have recently reported that pyrenyl-terminated *n*-alkanethiolate significantly rectifies tunneling currents in large-area junctions of liquid metal top-contact comprising eutectic gallium-indium. In this presentation, we demonstrate that the on-surface supramolecular structure of the pyrenyl terminal moiety critically determines the electronic function of molecular diode that relies on the second-order Stark effect. Specifically, we reveal that the change in tilt angle of the pyrenyl terminal moiety with respect to the external electric field critically determines the degree of the second-order Stark effect and hence the rectification ratio of the diode.

Poster Presentation : **MAT.P-435**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Biomimetic Signal Transduction Cascade using Pro-Nanozyme for Enzyme Activity Assay

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In the intracellular signaling system, initial stimulus amplifies huge signals through the chemical cascade reactions called signaling transduction pathway, activating related pro-enzymes. However, mimicking the signal transduction cascades for biosensor systems is challenging due to the complex design of the artificial pro-enzyme that can be activated by specific stimuli. Herein, we present the sequential signal transduction for enzyme activity assay using the amphiphilic nanozyme and the biphasic reaction system. In the water layer, when one of the nanozymes that loaded hydrophobic catalysts recognizes the specific signal, it delivers the tens of the catalysts to the oil layer including pro-fluorophore molecules, transducing the stimuli to the catalysts. The delivered catalysts convert the pro-fluorophore to the fluorophore, amplifying the catalytic signal to the optical signal. The potential of this assay mimicking intracellular signal transduction cascade was demonstrated through the monitoring of activity of Caspase 3, establishing the artificial signal transduction platform for both diagnosis and drug screening.

Poster Presentation : **MAT.P-436**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of N-Doped Carbon-Coated Cobalt Oxide from MOF as an Anode Material for Li-Ion Batteries

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Lithium-ion batteries (LIBs) have been widely used as energy storage materials in various electronic devices due to high energy density, long life cycle, and light of weight. However, graphite as a commercial anode material for LIBs has a problem such as low theoretical capacity (372 mAh g^{-1}). Recently, cobalt (II, III) oxide (Co_3O_4) is considered as an alternative anode material for high-performance LIBs because of its high theoretical capacity (890 mAh g^{-1}). However, Co_3O_4 anode materials suffer from low conductivity and poor cycle life due to structural strain and huge volume change during lithiation/delithiation processes. In this work, N-doped carbon embedded porous Co_3O_4 nanoparticles ($\text{Co}_3\text{O}_4/\text{NC}$) were synthesized by using Zn and Co metal-organic frameworks templates (ZIF-8@ZIF-67) and dopamine as a nitrogen and carbon source. During the synthesis, Zn species was evaporated to form the structural pores, and the in situ formed Co(0) catalyzed the graphitization of N-doped carbon matrix and transformed to Co_3O_4 . The $\text{Co}_3\text{O}_4/\text{NC}$ exhibited the improved discharge capacity of about 1177 mAh g^{-1} at 0.1 C rate after 50 cycles in voltage ranges of 0.01-3.0 V, which is superior to that of bare Co_3O_4 (719 mAh g^{-1}).

Poster Presentation : **MAT.P-437**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Guanidinium-Incorporated Cesium Lead Halide Perovskite for Green-Light-Emitting Diodes

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Organic-inorganic lead halide perovskites have attracted much attention as promising candidates for photovoltaics (PVs), light-emitting diodes (LEDs), and lasing materials due to their excellent optical and electronic properties, high color purity, and their widely tunable emission wavelength. Cesium (Cs)-based lead halide perovskites have received much attention as light emitting materials due to their excellent photoelectronic properties. Despite the high efficiency for light emitting diodes (LEDs), only a few cesium lead bromide (CsPbBr₃) perovskite-based devices have been developed due to the low stabilities and/or the formation of undesirable phase under ambient condition. Herein, it is demonstrated that a small quantity of guanidinium (GUA) A-site cation addition results in enhanced photoluminescence and improved crystallinity of the perovskite films. A GUA-incorporated multi-dimensional quasi-2D film with higher photoluminescence quantum yield (~20%) than Cs-only 3D perovskite film (~10%) was employed in a green-LED device with an inverted structure of glass substrate/indium tin oxide (ITO)/zinc oxide (ZnO)/poly(ethyleneimine) (PEI)/perovskite/poly(4-butylphenyl-diphenyl-amine) (poly-TPD)/WO₃/Al. With an addition of GUA A-site cation, we achieved much higher brightness and current efficiency of ~10000 cd m⁻² and 9.0 cd/A in the LEDs of perovskite thin film as compared to Cs-only perovskite thin film LEDs with ~400 cd m⁻² and 0.2 cd/A.

Poster Presentation : **MAT.P-438**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhanced Water Oxidation Efficiency with Polarized Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O₃ Perovskite Electro-Catalysts

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The water oxidation reaction, half reaction of water splitting, is considered as a major huddle for achieving spontaneous water splitting due to its sluggish kinetics and instability of catalysts in oxidation process. To overcome these problems, a lot of efforts are made on developing non-noble metal based water oxidation catalysts. Metal oxides with cation and oxygen vacancy have been considered as a strong candidate due to its abundancy and decent activity. Among the metal oxides, perovskites (ABO₃) have gotten great attention due to tunable catalytic activity by changing chemical compositions. In this study, we present synthesized cubic phase Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O₃. (denoted as BSCF) with polarization using external high voltage. The poled BSCF shows increased oxygen vacancy on surface of electrode caused by polarization. At electro chemical analysis the current density for OER could be enhanced by 33.7 mA/cm² at 1.8 V vs. RHE.

Poster Presentation : **MAT.P-439**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Intercalation of Cobaltocene into WS₂ Nanosheets for Enhanced Catalytic Hydrogen Evolution Reaction

**In Hye Kwak, Ik Seon Kwon¹, Jaemin Seo¹, Jisun Yoo¹, Kim Doyeon¹, Jong Hyun Lee¹,
Jeunghee Park^{1,*}**

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

We synthesized cobaltocene (7-20%)-intercalated WS₂ nanosheets using a solvothermal process. The intercalation of cobaltocene between the expanded 1T' phase WS₂ layers was confirmed by scanning transmission electron microscopy and electron energy loss spectroscopy. The intercalated complexes exhibit excellent performance for catalytic hydrogen evolution reaction (HER), with Tafel slope of 40 mV dec⁻¹ and 10 mA cm⁻² at 0.17 V (vs. RHE). Spin-polarized density functional theory calculations showed that cobaltocene is intercalated in the parallel orientation of fivefold symmetry to WS₂ plane, forming the charge-transfer complex. Reaction pathway calculations suggest that the basal S atoms just above the Co are the active sites, and the activation barrier of the Heyrovsky reaction determines the catalytic activity.

Poster Presentation : **MAT.P-440**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Scanning Transmission Electron Microscopy of Two-Dimensional Transition Metal dichalcogenide-Molecules Intercalated Nanosheets

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Two-dimensional layered structures have recently drawn worldwide attention because of their intriguing optical, electrical, and catalytic properties. Molybdenum disulfide (MoS₂) and tungsten disulfide (WS₂) are considered as the most promising catalysts for water-splitting hydrogen evolution reaction (HER) to replace the expensive Pt. MoS₂ and WS₂ nanosheet exhibits polymorphic phases such as stable semiconducting 2H (trigonal prismatic) phase, metastable metallic 1T phase, and metastable 1T' (distorted 1T) semi-metallic phase, depending on the synthesis procedure. Many strategies have been developed to maintain the metastable 1T or 1T' phase by controlling its electronic structures. We found that the intercalation of amine molecules is a promising strategy to enhance the stability of 1T' phase MoS₂ nanosheets and their HER performance. To directly observe the 1T' phase and the intercalated molecules, high-angle annular dark-field scanning (HAADF) and annular bright-field (ABF) imaging mode in an advanced (spherical) aberration-corrected high-resolution scanning transmission electron microscopy (STEM) was employed. The ABF-STEM image recognizes light atoms such as carbon of intercalated molecules. Electron-energy loss spectroscopy (EELS) across the interlayers was taken to show the elements between the expanded layers.

Poster Presentation : **MAT.P-441**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

TMD Materials@Si nanowire Photocathode as Effective Photoelectrochemical Hydrogen Evolution Reaction Catalyst

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Photocatalysts for hydrogen production are in demand because it is promising renewable energy technologies to handle environmental problem and depletion of fossil fuel. Even scientists put tremendous effort, sumptuary electrode catalysts with high activity remains a great challenge. In this work, we report transition metal dichalcogenide (TMD) nanosheet as an effective photocatalyst for water-splitting reactions. We fabricated TMD photocathodes onto a p-type Si nanowire array, which is 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-442**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Two Dimensional MoS₂/Fe-Phthalocyanine Hybrid Nanosheets as Excellent Bifunctional Electrocatalysts for Hydrogen Evolution and Oxygen Reduction Reactions

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¹*Micro Device Engineering / Microdevices, Korea University, Korea*

Two-dimensional layered MoS₂ has recently been considered as an excellent catalyst for water-splitting hydrogen evolution reaction (HER). Herein, we report that two dimensional MoS₂ and Fe-phthalocyanine hybrid nanostructures exhibit excellent bifunctional catalytic activity toward the HER and oxygen reduction reactions (ORR). The catalytic HER is characterized by a Tafel slope of 32 mV dec⁻¹ and 10 mA cm⁻² at an overpotential of 0.12 V. The number of electrons involved in the ORR was 4. The remarkable bifunctional performance would be ascribed to a synergic effect of electron-rich metallic 1T' phase MoS₂ and the active Fe-N₄ sites toward ORR. Spin-polarized density functional theory calculations on reaction pathway of HER suggests that the basal S atoms just above the Fe are active sites and the catalytic activity is determined by the activation barrier of Heyrovsky step.

Poster Presentation : **MAT.P-443**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Characterization of Unexploited IV-V Layered Structures

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The recent discovery of graphene has given rise to significant an interest in searching for new two- as GeP, GeAs, SiAs, and GeAs₂ using the exfoliation of bulk crystals that were synthesized by Bridgeman melt-growth method. A tip sonication of bulk crystal in N-methyl pyrrolidine (NMP) produced thin nanosheet to show the dramatic increase of the optical band gap, which is in the visible-light range of 2.1-2.3 eV. dimensional (2D) materials with their three-dimensional prototypes, where the 2D layers are stacked with weak van der Waals interactions. One of the remarkable properties of the 2D nanostructures is their unique quantum confinement effect at the 2D limit. As new potential class of 2D materials, IV-V MX_x compounds (M = Si, Ge, Sn, Pb; X = P, As, Sb, Bi; x = 1-3) have been recently proposed from theoretical calculations. The E_g of their monolayer can reach 2 eV, whereas that of the bulk is below 1 eV. In the present work, we synthesized the MX_x nanosheets such These band gaps are in a remarkable agreement with the theoretical prediction. We demonstrated that the nanosheets deposited n-Si nanowire arrays can be a promising photoanode for visible-light-driven water splitting.

Poster Presentation : **MAT.P-444**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of Wide Bandgap GeP Nanosheets and Their Electrical Properties

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¹Advanced Materials Chemistry, Korea University, Korea

Since the finding of graphene, there has been growing interest in new two-dimensional (2D) materials, where the 2D layers are stacked via weak van der Waals interactions. The reduction of a materials' dimension from bulk (3D) to 2D results in remarkable optical and electrical properties such as the increase of band gap and carrier mobilities due to the quantum confinement effect. Binary IV-V, where IV is Si, Ge, Sn, Pb and VI is P, As, Sb, Bi, have recently been emerged as another potential class of 2D materials. In the present work, we synthesized 2D GeP nanosheets using mechanical exfoliation method. A tip sonication of bulk crystal in N-methyl pyrrolidine (NMP) produced thin nanosheet to show the increase of the band gap, which is about 2.3 eV. First-principles calculations were performed to predict a significant increase of E_g when the number of layers decreases, and an indirect E_g of 2.3 eV for the monolayer. Field-effect transistor was fabricated to show the significant decrease of hole mobility but the increase of on-off ratio as the layer number decreases. We also observed in-plane anisotropic factor. The larger on-off ratio (104) for the thinner ones promises novel 2D (photo)electronic nanodevices.

Poster Presentation : **MAT.P-445**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Surface Enhanced Raman Spectroscopy at Nanogap between Au Nanoparticles Separated by 2D hexagonal Boron Nitride

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Department of Chemistry, Chonnam National University, Korea

The controlled formation of hot spot formed at nanogap between metal nanoparticles in surface enhanced Raman spectroscopy (SERS), since it can enhance the Raman signal of target molecule dramatically. Therefore, various methods have been attempted to produce the nanogap, and several approaches even enable the single molecule level detection by SERS. Nevertheless, the precise control of nanogap is not only technically difficult, but also the reproducibility is not good. In addition, the most of approaches are not appropriate for practical applications. Herein, we present a new approach to produce nanogaps between Au nanoparticles (Au NPs) separated with hexagonal boron nitride (h-BN) by making a Au NPs/h-BN/Au NPs heterostructure. In previous study, we have demonstrated that h-BN can be a good wrapping layer for SERS nanoparticle, which is used as a two-dimensional insulator material. The Au NPs/h-BN/Au NPs heterostructure can be manufactured by introducing additional Au NPs onto h-BN/Au NP substrate. The theoretical simulation has been carried out by using Finite-Difference Time-Domain (FDTD) method to visualize the electromagnetic field amplification at Au NPs/h-BN/Au NPs nanogap, which reveals that the stronger electromagnetic field can be generated at the nanogap structure of AuNP/h-BN/AuNPs. We believe that our results provide the critical insight for the nanogap based SERS applications by using the heterostructures of two-dimensional insulators and metal nanoparticles.

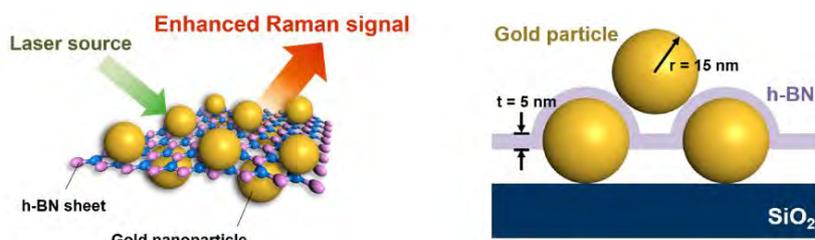


Figure 1. Schematic illustration of Au nanoparticles/h-BN/Au nanoparticles heterostructure

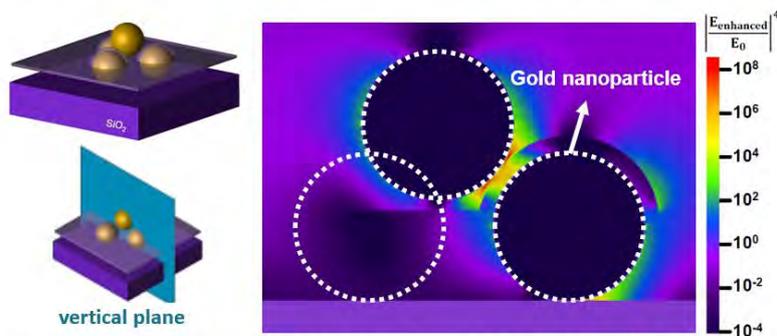


Figure 2. Finite-Difference Time-Domain simulation results of Au nanoparticles/h-BN/Au nanoparticles structure



Poster Presentation : **MAT.P-446**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solvent-free synthesis of metal nanoparticles and reduced graphene oxide composite for EMI shielding

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We report a novel method to synthesize composites of metal nanoparticles (NPs) and reduced graphene oxide (RGO) sheets, which were prepared by solvent-free reaction among corresponding metal precursor, graphene oxide (GO), and solid hydrazine ($\text{H}_3\text{N}+\text{NHCO}_2^-$). The synthesized composites were fully characterized by X-ray diffraction, transmission and scanning electron microscopy, IR spectroscopy, Raman spectroscopy, thermogravimetric analysis, electrical conductivity, and electromagnetic interference (EMI) shielding analysis. All the synthesized metal NPs/RGO composites were mixed with acryl resin to their EMI properties. The EMI shielding test was measured with a coaxial holder and network analyzer in the frequency range 1-6 GHz at 25 °C. An excellent EMI shielding efficiency was obtained at 5.2 GHz. Details on the fabrication of the composites and their properties will be presented.

Poster Presentation : **MAT.P-447**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Calcium-Doping for Structure Stabilization of Sodium Transition Metal Oxide Cathodes in Sodium Ion Batteries

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P2-Na_{0.67}Ni_{0.33}Mn_{0.67}O₂(NNMO), which has a layered structure, is a promising cathode material for sodium ion batteries. The stack TM slabs in a layered structure of NNMO, are composited of edge and face-shared (TM)O₆ octahedra, forming metal-occupied Octahedral sites and empty tetrahedral sites. The prismatic sites in Na slabs are also occupied by Na⁺ ions, which are sandwiched by edge and face-sharing with TM slabs. In this work, P2-Na_{0.67-2x}Ni_{0.33}Mn_{0.67}O₂ (0 < x ≤ 0.1) was synthesized by incorporating Ca²⁺ into NaO₆ layer of NNMO. Both the significant difference in ionic radii between Ca²⁺ (1.0Å) and Ni²⁺ (0.69 Å), Mn³⁺ (0.58 Å) and the reduction of Na⁺ content allowed the preparation of phase-pure and cation-mixing-free (i.e., absence of Ca²⁺ in transition metal oxide layers) Na_{0.67-2x}Ca_xNi_{0.33}Mn_{0.67}O₂ up to x = 0.05. It is expected that, while no noticeable change is observed in a dimension of (TM)O₆ octahedron, NaO₆ layers continuously shrink as the increase of Ca²⁺ content. The latter effect was expected to prevent the structural change (Na⁺-vacancy ordering) during repeated charge-discharge, eventually contributing to the improvement of capacity retention. Preliminary study indicated that, while pristine NNMO. showed a continuous decrease in discharge capacity, Na_{0.57}Ca_{0.05}Ni_{0.33}Mn_{0.67}O₂ maintained a significant fraction of an initial capacity with a small capacity fading during 40 cycles.

Poster Presentation : **MAT.P-448**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

B₃S Honeycomb Monolayer with High Specific Capacity for Lithium-Ion Batteries

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Igniting discovery of graphene stimulated the passion to investigate two-dimensional (2D) materials. The atomically thin material has unique electronic, optical and mechanical properties. Such fascinating properties lead to vast applications in the field of energy storage, photocatalysis, electrocatalysis etc. Here, we will present a proposed new binary compound with a unique electronic configuration, flexible bonding ability, and a relatively low symmetric honeycomb structure: monolayer B₃S. The designed new monolayer is dynamically, mechanically and thermally stable with high cohesive energy. This material has the highest Li storage capacity (1662 mA h g⁻¹) among the reported 2D monolayer so far. The low open-circuit voltage (0.16 V) and Li-diffusion barrier (< 0.4 eV) make the B₃S monolayer as an appealing candidate for the anode material in lithium-ion batteries.

Poster Presentation : **MAT.P-449**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

High Photocatalytic Degradation of Organic Dyes by GO/HNTs/ZnO Nanocomposites under Visible Light Irradiation

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ZnO is a semiconductor material with a wide bandgap of 3.4 eV and large exciton binding energy of 60 meV. It also shows optical activity and no photocorrosion effect. With these properties, numerous reports have been studying photocatalytic degradation of organic dyes using ZnO as a catalyst under visible light irradiation. 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. Due to these properties, we have found that ZnO effectively adsorbed on the surface of HNTs. HNTs prevent aggregation of ZnO and bring photocatalytic synergy effect. Graphene oxide (GO) consists of hexagonal carbon atoms to sp^2 bonds. It has features for photocatalytic application including high surface area, high thermal stability and excellent electron mobility. Taking these advantages, HNTs/ZnO nanocomposites grown on GO are thermally stable during photocatalyst. The photocatalytic degradation of methyl orange (MO) by ZnO and synthesized GO/HNTs/ZnO was compared under visible light irradiation. It was found that photocatalytic degradation ratio of MO using ZnO for 120 min reached 35%, whereas the degradation ratio of MO using GO/HNTs/ZnO for 120 min reached 95%, suggesting that these nanocomposites remarkably enhance the photocatalytic degradation of MO. In addition, we found that these nanocomposites show excellent photocatalytic capability and recycle stability during four cycles.

Poster Presentation : **MAT.P-450**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of an Improved Surface Coating Reagent Compared to Dopamine

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Catecholamine surface chemistry has received a great deal of attention due to its universal coating property. Catechol oxidation and intramolecular cyclization underlie the unique property of catecholamine surface chemistry. Based on these inspiring properties, a fast and universal surface chemistry technique using a new catecholamine is reported herein. A simple change in chemical structure of dopamine gives rise to the significantly accelerated intermolecular assembly and surface coating. The effect of catechol conjugation on a functional polymer coating is also investigated. The use of new catecholamine instead of dopamine to make polysaccharide coating materials improves the coating rate while maintaining the intrinsic property of the coated surface.

Poster Presentation : **MAT.P-451**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Calcium storage in graphite anode and organic cathode: Implementation in a rocking chair type calcium ion battery

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Despite significant improvement in electrolyte systems during the past few decades, divalent ion (Mg^{2+} and Ca^{2+}) batteries still suffer from electrolyte-incompatibility with metallic anodes. We propose graphite as a reliable Ca^{2+} -intercalation anode in tetraglyme (G_4). When charged (reduced), graphite accommodates solvated Ca^{2+} -ions ($Ca-G_4$) through intercalation and delivers a reversible capacity of 62 mAh g^{-1} forming a ternary intercalation compound, $Ca-G_4 \cdot C_{72}$. Mass/volume changes during $Ca-G_4$ intercalation and the evolution of in-operando X-ray diffraction studies both suggest that $Ca-G_4$ intercalation results in the formation of an intermediate phase between stage-III and stage-II with a gallery height of 11.41 \AA . Density-functional-theory calculations also reveal that the most stable conformation of $Ca-G_4$ has a planar structure with Ca^{2+} surrounded by G_4 , which eventually forms a double stack that aligns with graphene layers after intercalation. Despite large dimensional changes during charge/discharge (C/D), both rate performance and cyclic stability are excellent. Graphite retains a substantial capacity at high C/D rates and shows no capacity decay during as many as 2000 C/D cycles. As the first prototype Ca^{2+} -shuttling calcium-ion batteries (CIBs), a full-cell consisting of a Ca^{2+} -loaded graphite anode and an organic cathode is also constructed, and its electrochemical performance is presented. We hope that this work helps pave the way for the development of commercially viable CIBs.

Poster Presentation : **MAT.P-452**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Rechargeable Mg-Ion Battery: An Organic Electrode Material for High-Voltage MIB's

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Magnesium-ion batteries (MIB's) can be an attractive alternative for grid-scale energy storage due to the abundance of Mg resources. Mg-ion battery has attracted much attention in the past two decades due to its high theoretical volumetric capacity (3833mAh/cm^3) compared to lithium-ion battery [850mAh/cm^3 (Graphite anode)]. Magnesium possesses two valence electrons and has a low standard reduction potential (-2.37 V vs. SHE). Until now only inorganic materials have been reported as anodes in Mg-ion batteries compatible only with Grignard type electrolytes. The dendrite free nature of Mg is amenable for assembling high voltage and high energy density batteries with suitable cathode materials, but the passivating behaviors of the Mg in carbonate type electrolytes make it irreversible. Organic electrode materials could be highly promising alternatives for inorganic counter-part. The organic materials are structure contrivable and environmentally benign achieving high gravimetric energy density and cycling stability in battery applications. In this work, magnesium perylene-3,4,9,10-tetracarboxylate ($\text{Mg}_2\text{-PTC}$) was synthesized starting from perylene-3,4,9,10-tetracarboxylic acid-dianhydride (PTCDA). The Mg_2PTC was characterized by XRD and other techniques to confirm the target molecule structure. Further, the electroactivity of $\text{Mg}_2\text{-PTC}$ was tested in carbonate type electrolyte by several electrochemical methods. Detailed electrochemical and spectroscopic investigations of the $\text{Mg}_2\text{-PTC}$ are underway.

Poster Presentation : **MAT.P-453**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Improve Stability and Reduce Hysteresis of Perovskite Solar Cell with F4-TCNQ as a P-type Dopant for Polymer Hole-Transporting Material

Hannah Kwon, Dong Ha Kim*

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Perovskite solar cells (PSCs) have drawn significant attention and opened up a new prospect in the photovoltaic technologies to address the contemporary energy and environmental issues. Designing a hole transport material (HTM) is regarded as one of the most important approaches to improve the efficiency and stability of PSCs. Herein, an efficient model is suggested by optimizing the conjugated polymer, TFB (Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(4,4'-(N-(4-sec-butylphenyl)diphenylamine))]), and non-hygroscopic p-type dopant F4-TCNQ (2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane). TFB-doped F4-TCNQ can be an ideal alternative to conventional HTM to realize low price, high hole mobility and suitable energy band alignment with perovskite material. The combination of highest occupied molecular orbital (HOMO) level of TFB and lowest unoccupied molecular orbital (LUMO) level of F4-TCNQ was believed to favor an efficient charge and energy transfer between perovskite and hole transport layer (HTL), and to reduce charge recombination. Consequently, the combined utilization of the TFB and F4-TCNQ could enhance photoconductivity to improve power conversion efficiency, which resulted in the superior stability of the perovskite solar cells. This simple, novel strategy demonstrates a promising route to improve the performance of the HTL and its application to a wide range of solar cells and other photovoltaic applications.

Poster Presentation : **MAT.P-454**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Free-standing MnCoO_x@NCNF anode material for Li-ion battery

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Herein, a smart strategy is proposed to tailor unique interwoven nanocable architecture consisting of MnCoO_x nanoparticles embedded in 1-dimensional (1D) mesoporous N-doped carbon nanofibers (MnCoO_x@NCNFs) for the first time by using electrospinning technique. As-prepared MnCoO_x@NCNF composite is tested as a current collector-free and binder-free flexible anode, which eliminates slurry preparation process during electrode fabrication in Li-ion battery (LIB). They possess versatile structural characteristics which can address simultaneously different issues such as poor conductivity, low cycling stability, volume variation, flexibility, and binder issue associate with the metal oxide, and thus enable not only high initial discharge and charge capacities but also reversible discharge cycling stability of almost 80 % retention up to 100 cycle and 60 % retention up to 500 cycles at 1 A/g. Such high Li storage capacity and excellent cycling stability are attributed to the unique flexible and free-standing spider network-like architecture of 1D MnCoO_x@NCNFs, which provides the platform to bicontinuous electron/ion pathways for superior electrochemical performance. Along with excellent electrochemical performance, simple synthesis procedure of unique binder-free MnCoO_x@NCNFs can achieve cost-effective scalable mass production for practical use in flexible mode, not merely in LIBs but also in a wide spectrum of energy storage fields.

Poster Presentation : **MAT.P-455**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication of High Performance Hole Transporting Layers based on MoS₂/PEDOT:PSS Hybrids for Organic Solar Cells

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

In recent years the massive increase of environmental pollution and global warming due to vast consumption of fossil fuels, has led researchers to intensify and focus on the study of renewable energy sources. Solar energy has emerged as the favorable solution for sustainable development. Organic Solar Cells (OSCs) have been considered as one of the most promising solar cell technologies because of their many striking properties such as solution processability, light weight, flexibility, and simple manufacturing process. In OSCs, the charge transporting layers plays an important role for determining the power conversion efficiency. In this work we report the fabrication of hybrid hole transporting layer (HTL) based on solution-processed MoS₂ nanosheets and PEDOT:PSS for OSCs. As a strategy, we incorporated oleylamine functionalized 2D MoS₂ nanosheets into PEDOT:PSS for improving the surface properties of PEDOT:PSS and as well as enhancing the hole extraction from the active layer. We achieved power conversion efficiency up to 3.74% for P3HT:PCBM based OSCs employing the hybrid HTL, which is 15.08% higher than that of reference cells with neat PEDOT:PSS as HTL. Solution-processed MoS₂ nanosheets and hybrid HTL was characterized by range of complementary techniques such as Raman, UV-Visible, PL, AFM, TEM and impedance spectroscopy. We believe that the findings of this study can find significant importance in fabrication of 2D nanomaterials based HTL for OSCs.

Poster Presentation : **MAT.P-456**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Solution-Based Thermal-Aging Process of Vanadyl(IV)acetylacetonate Precursor for Deposition of VO₂ Thin Films and Their Optical Properties Control

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Thermochromic properties of vanadium dioxide (VO₂) have been studied extensively due to their IR reflection applications in energy smart windows. In this paper, we studied the optical switching property of VO₂ thin film, depending on the thermal aging time of the vanadyl(IV)acetylacetonate (VO(acac)₂) precursor. We found the alteration of the IR spectra of the precursor by tuning the aging time as well as heat treatments of the precursor. An aging effect of vanadium precursor directly affects the morphologies, optical switching property and crystallinity of VO₂ films. The optimum condition was achieved at the 7 day aging time with optical switching efficiency (E_{os}) of 50 %. Furthermore, we demonstrate the adjustment of optical properties of VO₂ thin films by nanosphere template assisted patterning process. Pattern sizes of films were varied as a function of the diameter of polystyrene (PS) spheres, and the size of the obtained films were 550, 900, and 1230 nm, respectively. The crystal structure of prepared films is a monoclinic phase of VO₂ (M), and there are no impurities or other oxides. The transmittance curve change was observed for all patterned VO₂ thin films, and it is strongly correlated with pattern sizes and shapes which can make a difference in the photonic band gap. In addition, it is found that such a transmittance curve change originated from reflection at a certain wavelength section which can be confirmed by reflectance spectra.

Poster Presentation : **MAT.P-457**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Highly Emissive Octahedral Rhenium Metal Cluster with Massive Stokes shift and Its Application on Transparent Luminescent Solar Concentrator

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The LSC is a device that employs luminescent dyes to concentrate the sunlight on PVCs (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 with high stability. 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, $(\text{Bu}_4\text{N})_4[\text{Re}_6\text{S}_8(\text{NCS})_6]$ and $(\text{dMDAEMA})_4[\text{Re}_6\text{S}_8(\text{NCS})_6]$ were prepared by reaction of $(\text{Bu}_4\text{N})_4[\text{Re}_6\text{S}_8\text{Cl}_6]$ with molten KSCN and dMDAEMAI 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-458**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhanced Performance of Inverted Organic Solar Cells by engineering Electron Transfer Layer.

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Organic photovoltaics (OPVs) have achieved high power conversion efficiency (PCE) by novel materials and advanced processes. In this work, we used ZnO and poly[(9,9-bis(3'-((N,N-dimethyl)-N-ethylammonium)-propyl)-2,7-fluorene)-alt-2,7-(9,9-dioctylfluorene)] (PFN) as electron transport layers (ETLs) for the inverted OPVs. The ZnO serves as an efficient ETL for reduced series resistance and the PFN improves energy alignment of devices. We found that the OPVs using both ZnO and PFN have higher performance than ZnO- or PFN- only devices. Our results could be one of the guidelines for more efficient OPVs.

Poster Presentation : **MAT.P-459**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile Fabrication of Hemisphere Film for Enhancing Solar Cell Efficiency Economically

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Solar cell has been commonly used as the next-generation power conversion device for several decades. It has competitive advantages due to infinite energy resource and eco-friendly industry. However, solar cell has critical demerits including low power conversion efficiency and economical effectiveness. In this study, we developed attachable thin film which has hemisphere pattern via nanoimprinting technique for overcoming those issues. In order to improve the low power conversion efficiency, we fabricated attachable hemisphere patterned film as an anti-reflection nanopatterns. Through combination of solar cell with hemisphere patterned film, we achieved the 10% higher power conversion efficiency.

Poster Presentation : **MAT.P-460**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhancement of solar cell efficiency by mixed spectral conversion materials

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We demonstrate the novel photonic structure doped with spectral conversion materials to enhance the solar cell efficiency by converting near-infrared (NIR) and ultraviolet (UV) to visible light, simultaneously. The periodically manipulating complex consisted by the dielectric matrix allows the localization of electric (E)-field due to guided-mode resonance and amplifies the absorption within a broad-band wavelength region. The proposed structure was fabricated using the direct imprinting technique that facilitates practical applications for optoelectronic devices.



Poster Presentation : **MAT.P-461**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Improvement optical properties of Perovskite quantum dots(PQD)- embedded SiO₂ film via nanoimprinting

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The Perovskite Quantum dots(PQD) have been studied due to its special down-shifting ability from UV region to Visible region. Especially, PQD shows unique characterizations; narrow-band emission spectra and high photoluminescence quantum yield, which are essential characters for various fields including industry and spectroscopy. However, applications of PQD to other fields require the transparency and enhanced optical performance. In this study, we fabricated advanced nanophotonic device using CsPbBr₃ PQD in order to optimize its intrinsic optical properties. With PQD-embedded SiO₂ films, we achieved enhancement of photoluminescence property of PQD maintaining its transparency.

Poster Presentation : **MAT.P-462**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Thermoelectric Properties of Cu_2SnS_3

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The thermoelectric (TE) materials have attracted much attention due to needs for potential renewable energy source. The efficient of thermoelectric devices can be evaluated by the figure of merit, $ZT = S^2\sigma T/\kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature and κ is the thermal conductivity. Among the various kinds of thermoelectric materials, sulfide materials regarded as a promising eco-friendly TE material due to their earth abundant, low-cost and non-toxic elements. Ternary sulfide Cu_2SnS_3 has recently attracted attention as an outstanding p-type thermoelectric materials with band gap 0.7-0.9 eV. In this study, we synthesize metal-doped Cu_2SnS_3 through solid state reaction. We consolidated metal-doped Cu_2SnS_3 to pellets with hot press. The crystal structure was investigated with X-ray diffraction and thermoelectric properties by ZEM-3 equipment (Ulvac-Riko) and NETZSCH LFA 457 MicroFlash™.

Poster Presentation : **MAT.P-463**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Horizontally Stacked Cobalt-Nickel Hydroxide Nano-crystals on Ni Foam as Electrode Materials for High Performance Pseudocapacitor

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A facile one-step method of synthesizing monolayered cobalt-nickel hydroxide nano-crystals ((Co, Ni)(OH)₂) is presented using ammonia transfer method in the closed vessel without exfoliation process. The electrode materials are fabricated by deposition of (Co, Ni)(OH)₂ on Ni metal substrate for 1 minute by electrophoretic deposition. Thin layer of (Co, Ni)(OH)₂ are deposited in average of 50 mg, showing brownish green color. The scanning electron microscope, transmission electron microscope and X-ray diffraction were used to analyze the morphology and crystal structure of (Co, Ni)(OH)₂ electrode. The electrochemical performance of (Co, Ni)(OH)₂ electrode with various molar ratio of cobalt and nickel as negative electrodes were characterized by cyclic voltammetry in KOH aqueous solution at room temperature.

Poster Presentation : **MAT.P-464**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

LiAl₂-LDH Grown in Anodic Aluminum Oxide Membrane for Lithium Adsorption

Yongju Lee, Duk-Young Jung*

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An LiAl₂-Layered Double Hydroxide (LDH)/Anodic Aluminum Oxide (AAO) membrane was synthesized on AAO in lithium chloride, ammonia solution to adsorb lithium cations. LiCl and ammonia solutions were passed through the AAO via a syringe pump for sufficient wetting of the interior of the AAO. The concentrations of ammonia and LiCl were controlled to find the optimal conditions for synthesis of LiAl₂-LDH/AAO. Thus, it was confirmed that LiAl₂-LDH/AAO was synthesized in LiCl, ammonia for 10 mins at 25°C. Under this condition LiAl₂-LDHs have just been formed on the inner AAO surfaces. The as-prepared samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM).

Poster Presentation : **MAT.P-465**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of heavily Cu-doped Bi₂Te₃ nanoparticles and their thermoelectric properties

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The thermoelectric (TE) materials are able to convert heat into electricity and have drawn increasing attention in several years due to the need for alternative energy of fossil fuels. The performance of thermoelectric materials can be evaluated by figure of merit ZT , which is defined as $\sigma S^2 T / \kappa$. Bi₂Te₃ and its derivative compounds are the most of studied thermoelectric materials and are widely employed in thermoelectric (TE) applications at room temperature. It is known that thermoelectric materials of nanostructure increase ZT relative to that of the bulk materials due to reduce the thermal conductivity without reducing the power factor. In this study, Cu-doped Bi₂Te₃ nanoparticle was synthesized by solution state reaction. The synthesized Cu-doped Bi₂Te₃ nanoparticles were consolidated by spark-plasma sintering into bulk pellets, and the thermoelectric properties (Seebeck coefficient and thermal conductivity) of these pellets were measured. Cu-doping in Bi₂Te₃ shows enhanced the Seebeck coefficient due to a decrease in carrier concentration, thus the power factors increased compared with that of the un-doped sample. As a result, Cu-doped Bi₂Te₃ sample with 15.6 at% Cu exhibits the best thermoelectric performance with a figure of merit of 0.67 at 415K.

Poster Presentation : **MAT.P-466**

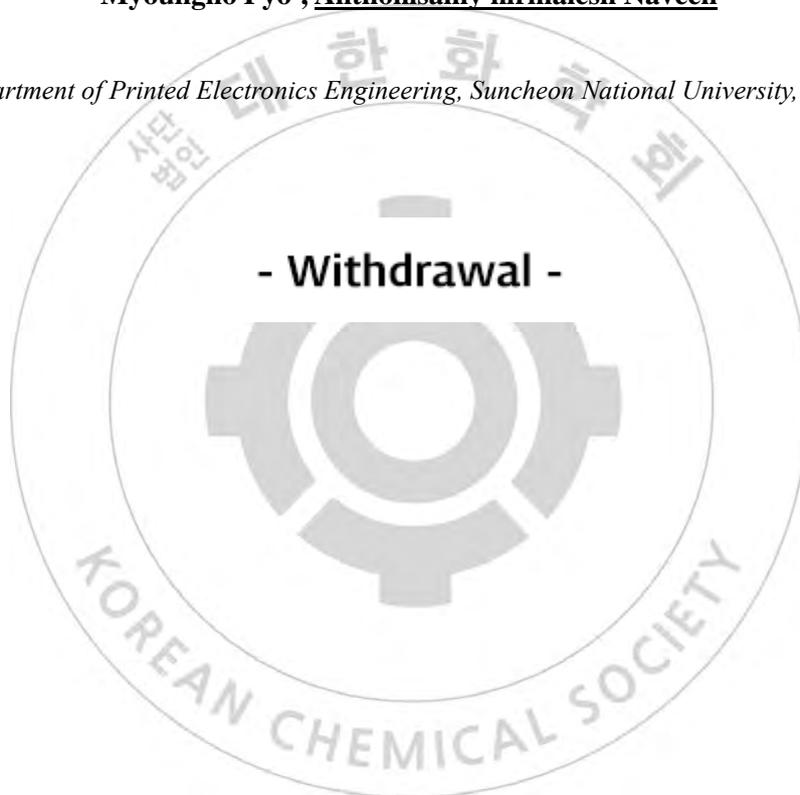
Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

[Withdrawal] Highly stable P³⁺-K_{0.8}CrO₂ cathode with limited dimensional changes for potassium ion batteries

Myoungho Pyo^{*}, Anthonisamy nirmalesh Naveen

Department of Printed Electronics Engineering, Suncheon National University, Korea



Poster Presentation : **MAT.P-467**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

FORMULATION OF NANO-COMPOSITE BIOINK FOR HEAT RESPONSIVE SOFT ACTUATOR

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Soft robotics is one of the new strategies in the field of medical treatment and pharmaceutical. Soft robotic can be applied for diagnosis tool and drug delivery to the specific tissue target. Soft robotic can be made using bio-3D printers using nano-composite as bio-ink which have a critical influence in properties and structure formed of the printed object. Therefore, it is able to maintain its shape and expected have good biocompatibility. Poly(N-isopropyl acrylamide) or PNIPAAm has the ability as photo-actuator due to its temperature-sensitive properties. PNIPAAm can shrink in above of lower critical temperature (LCST). The surface plasmon resonance (SPR) of a metal nanoparticle can be used as light into heat transfer initiator. The irradiation of light in the same wavelength with its SPR can initiate the light into heat transfer phenomena. Thus, PNIPAAm and metal nanoparticle properties to be employed as nano-composite bio-ink that has a potential for soft robotic photoresponsive material. In this study, the printability and mechanical properties of nano-composite bio-ink are evaluated through rheology and elasticity measurement by Young modulus test. Instead of those properties, the challenge of this study is to find out the best crosslinking agent by which the bio-ink has good elasticity and mechanical properties of the printed product. Furthermore, nano-composite bio-ink generated in this study high reproducibility, good properties and biocompatible.

Poster Presentation : **MAT.P-468**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Preparation and use of heterogeneous catalyst for olefin oxidation based on porous organic polymer support

Jongho Yoon, Suk Joong Lee*

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As the demand for various chemicals or polymers increases, the formation of carbon–oxygen bonds became one of the most critical process, and epoxide synthesis via olefin oxidation has become important. Because widespread olefin oxidation method using toxic reagents such as peracids inevitably produces explosive and toxic by-products, researchers have been focused on using transition metal catalysts such as vanadium, manganese, iron, and copper. These transition metal-based catalysts have high selectivity and efficiency, but their low stability and separation are still challenge. So, we synthesised bispyridine based POPs and immobilized of a CuCl_2 to prepare heterogeneous Cu-bpy catalyst for olefin oxidation. And it demonstrated great olefin oxidation as well as many advantages of easy separation, recycle possibility and high stability.

Poster Presentation : **MAT.P-469**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Development of Highly Stable P2-type $K_x[Ni_{1/3}Mn_{2/3}]O_2$ Cathode with Excellent Rate Characteristics for Potassium Ion Batteries

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Potassium ion batteries (KIBs) have gained great attention for energy storage devices owing to the elemental abundance and the lower reduction potential of potassium ions. Layered $Na_{2/3}[Ni_{1/3}Mn_{2/3}]O_2$ has been extensively studied as cathode material for sodium ion batteries (SIBs) due to its high theoretical capacity (173 mAh g^{-1}). Both the P3- and P2- $Na_{2/3}[Ni_{1/3}Mn_{2/3}]O_2$ were investigated for sodium ion storage, among them the P2- $Na_{2/3}[Ni_{1/3}Mn_{2/3}]O_2$ exhibited better performance than P3 compound. Therefore, in the present work, we have made an attempt to synthesize P2- $K_{2/3}[Ni_{1/3}Mn_{2/3}]O_2$ by conventional solid state route but the P2 phase was not stabilized. Consequently, we prepared P2-type $K_x[Ni_{1/3}Mn_{2/3}]O_2$ cathode material from $Na_{2/3}[Ni_{1/3}Mn_{2/3}]O_2$ by an electrochemical ion exchange process. The $K_x[Ni_{1/3}Mn_{2/3}]O_2$ cathode delivered a specific discharge capacity of 81 mAh g^{-1} at a current rate of 0.5C. The material demonstrated good rate performance with 49 mAh g^{-1} at 15C. The cycling stability was also superior with 86% initial capacity retention after 250 cycles. The excellent cycling stability and rate performance could be attributed to the fast K^+ diffusion through the 2D framework.

Poster Presentation : **MAT.P-470**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Lattice Spacing-Induced Supramolecular Structural Effect on the Performance of Molecular Tunneling Devices

Gyu Don Kong, Seohyun Kang, Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

The on-surface supramolecular structure of molecules plays an important role in molecular-scale electronic devices and other systems. However, understanding such a role is a significant chemical challenge because the supramolecular structure often relies on weak intermolecular interactions such as van der Waals and π - π stacking. This presentation describes the fine-tuning of weak supramolecular interactions in self-assembled monolayers (SAMs) by varying the lattice spacing of anchoring moieties through the change of bottom electrode. We focus on large-area tunnel junctions formed with binary mixed SAMs comprising 2,2'-bipyridyl-terminated *n*-undecanethiolate (organic diode) and *n*-alkanethiolates of different lengths (non-rectifying diluent molecules). Junction measurements indicate that replacement of bottom electrode from silver to gold leads to remarkably opposite trends of rectification as the length of the diluent molecule is changed. Finally, we discuss the origin of the opposite rectification behaviors for the gold and silver electrodes based on the results obtained from further studies with near edge X-ray absorption fine structure (NEXAFS), static and dynamic contact angle goniometries, and reductive desorption experiments.

Poster Presentation : **MAT.P-471**

Material Chemistry

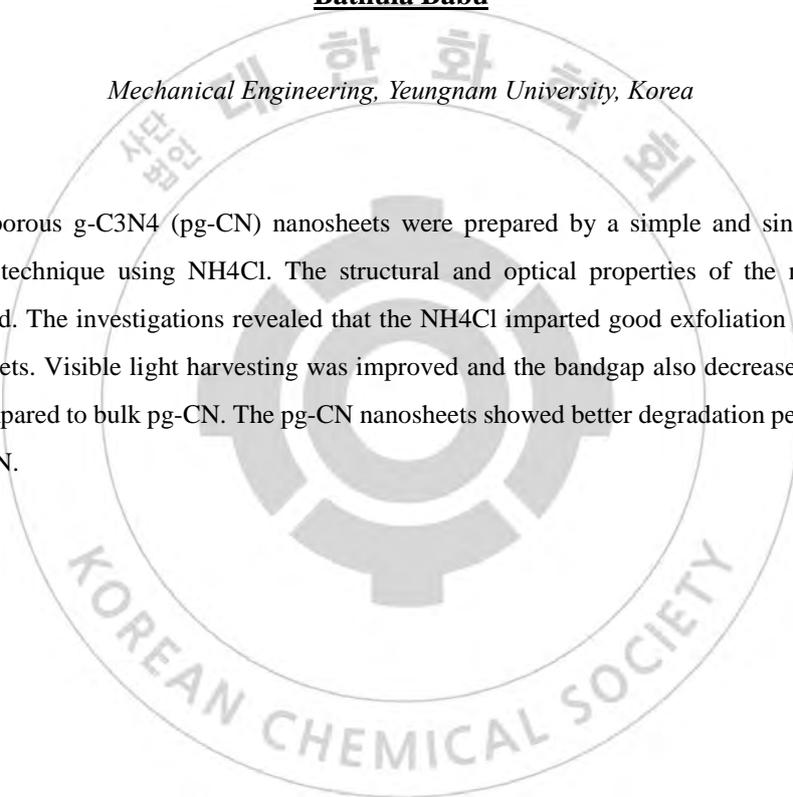
Exhibition Hall 2, FRI 11:00~12:30

Modification of porous g-C₃N₄ nanosheets for enhanced photocatalytic activity: In-situ synthesis and optimization of NH₄Cl quantity

Bathula Babu

Mechanical Engineering, Yeungnam University, Korea

In this study, porous g-C₃N₄ (pg-CN) nanosheets were prepared by a simple and single-step thermal decomposition technique using NH₄Cl. The structural and optical properties of the nanosheets were carefully studied. The investigations revealed that the NH₄Cl imparted good exfoliation properties to the pg-CN nanosheets. Visible light harvesting was improved and the bandgap also decreased for the pg-CN nanosheets compared to bulk pg-CN. The pg-CN nanosheets showed better degradation percentage of RhB over bulk pg-CN.



Poster Presentation : **MAT.P-472**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication and Characterization of CsPbBr₃@SiO₂ Perovskite Quantum-Dot Composites for ink-jet Printed Color Conversion Layer

Sang-Yoon Lee, Sol Choi, Jun Choi*

Human Convergence Technology Group, Korea Institute of Industrial Technology, Korea

Inorganic cesium lead halide perovskites (CsPbX₃, X = Cl, Br, I) have attracted enormous attention as a novel optoelectronic material with enhanced stability compared to the other perovskite materials. However, CsPbX₃ perovskite quantum-dot still contains the defects that the oxygen and moisture affect their stability and luminescence performance. Therefore, we have synthesized CsPbBr₃ quantum-dot/silica composites by applying silica for highly stable core-shell structures. The silica effectively passivated the perovskite quantum-dot composite surface, so it was able to maintain original high photoluminescence quantum yield in the air. We used low-speed centrifuged solution after the synthesizing process to make the printable inks. By using proper ink formulation recipe, we were able to set the suitable physical and rheological properties (viscosity, ink conductivity) of the inks for ink-jet printing process. We analyzed FT-IR, TEM image, XRD, optical properties, and color coordinates of the synthesized CsPbBr₃@SiO₂ particles and inks to verify their characters. The prepared CsPbBr₃ quantum-dot inks were ink jet printed, and formed the coated thin film which could be used as the color conversion layer of LED display. The prepared CsPbBr₃ quantum-dot inks and coated thin films exhibited excellent ambient stability and photoluminescence quantum yield with the efficient green emission.

Poster Presentation : **MAT.P-473**

Material Chemistry

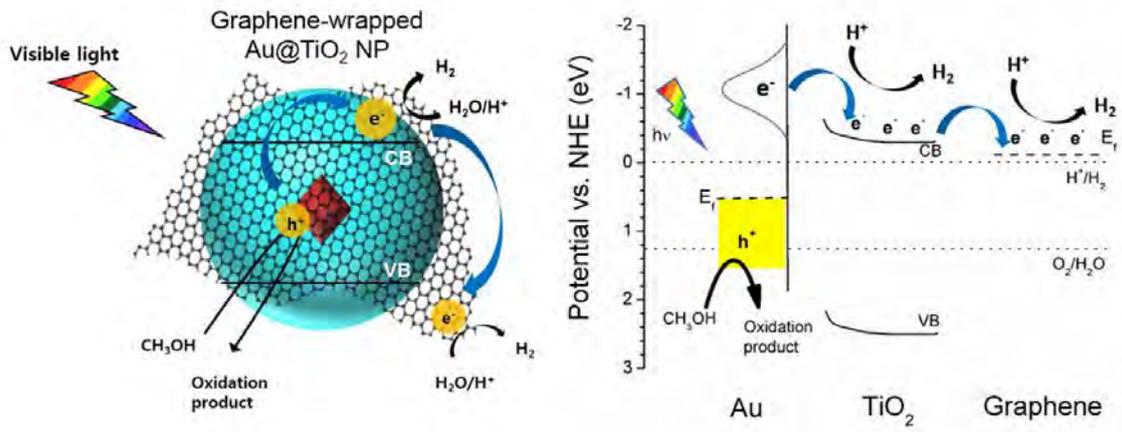
Exhibition Hall 2, FRI 11:00~12:30

Graphene Encapsulated Au@TiO₂ Core-Shell Nanostructures for Plasmon-Enhanced Photocatalytic Hydrogen Evolution

Hayoon Jung, Sang Woo Han*

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

There has been significant interest in heteronanostructures with controlled topologies and configurations for designing efficient photocatalysts. Herein, we present a promising solar energy conversion platform constructed by the intimate contact of graphene, semiconductors (TiO₂) and plasmonic metal nanocrystals (octahedral Au nanocrystals) with well-defined configurations. The complete wrapping of TiO₂ shell around Au nanocrystals and the sequential graphene encapsulation over TiO₂ shell were successfully realized by sol-gel processes, self-assembly methods, and post-calcination. Through core-shell engineering of the ternary hybrids, the plasmonic band of graphene encapsulated Au@TiO₂ core-shell nanostructures has redshifted from 550 nm to around 700 nm. Accordingly, the prepared nanostructures exhibited superior photocatalytic hydrogen production under visible light ($\lambda > 400$ nm) and red light irradiation ($\lambda = 700$ nm). A series of mechanistic studies on the photocatalysis indicated that the prominent photocatalytic activity of the hybrid nanostructures is attributed to the synergism between the hot electron transfer from Au nanocrystals and the efficient space separation of charge carriers by graphene. This study can provide new insights in designing heteronanostructures for visible and red light responsive photocatalysis.



Poster Presentation : **MAT.P-474**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Structural Studies of a New Mixed-valent Two-dimensional Quarternary Sulfide, $K_2Ta_6Pd_9S_{24}$

Sanghyun Bae, Hoseop Yun*

Department of Chemistry, Ajou University, Korea

The new quaternary sulfide, $K_2Ta_6Pd_9S_{24}$ has been synthesized from elemental powders through alkali metal halide flux methods and it is structurally characterized by single crystal X-ray diffraction techniques. The title compound crystallizes in the space group $I2/m$. Two crystallographically independent Ta atoms are found and they are surrounded by six S atoms in trigonal prismatic fashions. The Pd atoms are coordinated to four S atoms in square planes. These polyhedra are connected to form a two-dimensional layer, ${}^2_\infty[Ta_6Pd_9S_{24}{}^{2-}]$. These layers stack on top of each other and the K^+ ion reside between the layers to satisfy the charge neutrality. The charge valence of the title compound can be described as $[K^+]_2[Ta^{4+}]_2[Ta^{5+}]_4[Pd^{2+}]_9[S^{2-}]_{24}$. In this presentation, a comparison of the title compound with the previously prepared phases, $CsTaPd_3S_6$ and $Cs_2ZrPd_3S_6$ will be discussed.

Poster Presentation : **MAT.P-475**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Structural Characterization of a New 2-dimensional Chromium Thiophosphate, CsCr₃P₂S₁₀

Woojin Yoon, Hoseop Yun*

Department of Energy Systems Research, Department of Chemistry, Korea

The new 2-dimensional quaternary chromium thiophosphate, CsCr₃P₂S₁₀ has been prepared at high temperature via solid state reactions using CsI as a reactive flux. The crystal structure has been determined by single crystal X-ray diffraction techniques. The title compound crystallizes in the rhombohedral space group R-3m. The imposed symmetry of chromium atom is m and it is surrounded by six sulfur atoms in the octahedral geometry. Phosphorus atoms are coordinated by four sulfur atoms in the tetrahedral fashion. These polyhedra are combined to form the two-dimensional infinite anionic layer, ²⁻_∞[Cr₃P₂S₁₀], and alkali metal cations, Cs⁺ stay in the van der Waals space between the layers through electrostatic interactions to complete the three-dimensional structures. The classical charge valence can be described as [Cs⁺][Cr³⁺]₃[P⁵⁺]₂[S²⁻]₁₀.

Poster Presentation : **MAT.P-476**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Microwave-assisted synthesis of reduced Graphene oxide/Mn₃O₄ hybrids with spherical hollow structure for lithium-ion battery application

Seung-Min Paek*, **Min-Jae Kim¹**

Department of Chemistry, Kyungpook National University, Korea

¹*department of chemistry, Kyungpook National University, Korea*

Graphene has received enormous interests in electrochemical fields owing to its large specific surface area, and excellent electrical and mass conductivities. Thus, in this study, the graphene was hybridized with manganese oxide nanoparticles which has large specific capacity in lithium-ion batteries through layer-by-layer self-assembling on polymer template. And then, microwave was irradiated to the nanohybrids for modification of their physico-chemical properties such as surface area, porosity, electrical and mass conductivity for using the anodic materials in lithium-ion battery. According to the electron microscopy (SEM, TEM) images, the nanohybrids have spherical hollow structure. In the energy dispersive spectroscopy(TEM-EDS) mapping images, it was observed that the carbon and manganese oxide were homogeneously distributed in nanohybrids. In the electrochemical tests, the obtained nanohybrids had higher electronic conductivity, ion-diffusion property and specific capacity than the bare MRGO. The obtained nanohybrids could be used as anode materials in lithium ion batteries.

Poster Presentation : **MAT.P-477**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Geometry Isomer Effects of Terphenyl Backbone Based Donor-[-]-Acceptor Dyads on the Intramolecular Charge Transfer

Minji Kim, Kyung-Ryang Wee^{1,*}

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¹*Department of Applied Chemistry, Daegu University, Korea*

The geometry effects of ortho, meta, and para-terphenyl isomer structure on the intramolecular charge transfer (ICT) process of the donor (D)-[-]-acceptor (A) dyads (D-[-]-A) were studied to understand the structure-properties relationship. These terphenyl based D-[-]-A dyads were prepared by two-step palladium catalyzed Suzuki-Miyaura coupling reactions, consisting triphenylamine (TPA) as an electron donor and 1,2-diphenyl-benzimidazole (imi) units as an electron acceptor, respectively. The photophysical and electrochemical properties of the terphenyl backbone based ortho (**O**), meta (**M**) and para (**P**) dyads were compared with each other. In the steady state absorption spectra, a gradual red-shift property was observed in the order of **O** < **M** < **P** due to each terphenyl isomer conjugation effects. In particular, the emission spectra of the all of para-terphenyl D-[-]-A showed similar emission maximum of 475 nm and bathochromic shift property with increasing the solvent polarity, which is attributed to the ICT process. Emission quantum yields of the para-terphenyl D-[-]-A isomers were showed in the order of **P** ≥ **O** >> **M** and the emission lifetimes were recorded 7.85 (**O**), 11.6 (**M**) and 2.02 (**P**) ns in CH₂Cl₂, respectively. Based on experimental results, we assumed that **P** dyad is through bond ICT process, while **O** and **M** isomers are through space ICT process. In addition, the distance of the donor-acceptor of **M** dyad is larger than that of **O** dyad, resulting in slow through space ICT with a nonradiative quenching process. In the DFT/TDDFT calculations, this result is well agreed with experimental data.

Poster Presentation : **MAT.P-478**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Integrated Tandem p⁺n-Silicon-SnO₂/TiO₂ Photoelectrochemical Cell for Efficient Photoinduced Water Splitting

Minji Kim, Kyung-Ryang Wee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

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. 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. 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. 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 : **MAT.P-479**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optical and Magnetic Properties of Self-Doped Cd_xHg_{1-x}Se Alloy Nanocrystals

Dongsun Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

The researches of colloidal quantum dots (CQDs) focused on the bandgap transition for decades. The first steady state mid-IR intraband transition from the mercury system was reported by Jeong et al. in 2014. The recent research has substantiated that the self-doping property leads the intraband transition in the nanocrystal. In this poster, I will present the mid-IR photoluminescence and magnetism of self-doped Cd_xHg_{1-x}Se alloy nanocrystals. The CdHgSe alloy nanocrystals have the electronic transition progressively shift from visible to the mid-IR localized surface plasmon resonance (LSPR) by increasing the quantity of mercury substitution in the CdSe nanocrystals. The visible emission from nanocrystal is red shifted, and the average lifetime increased as Hg substituent ratio accretion. The further increment of the mercury ratio in the alloy change the major transition to the mid-IR region and successfully measured the mid-IR photoluminescence with the home-built mid-infrared spectrometer. Surprisingly, the mid-IR emissive alloy nanocrystal showed singly-occupied quantum-state from the EPR measurement, and free electron signal as the LSPR revelation, respectively. The photoresponsivity of the fabricated device also confirmed the LSPR development from the alloy nanocrystal. The self-doping study, therefore, gives the novel opportunity to research the change in the electron properties when the material character alters from semiconductors, semi-metals, to metals.

Poster Presentation : **MAT.P-480**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The Comparative Studies on Photophysical and Redox Properties of the Mononuclear and Dinuclear Ru(II) Complexes Prepared from the Photosensitizing Unit

Chang-Shik Choi

Department of Food and Nutrition, Far East University, Korea

Photo-induced energy or electron transfer processes in supramolecular species are currently the object of much interest in view of the design of photochemical molecular devices.¹ In particular, Ru(II) polypyridyl complexes have been frequently used as building blocks of polynuclear complexes that behave as supramolecular species. However, synthetically, it was found very difficult to assemble these metal complexes in a rigid and extended structure that could facilitate the migration of energy or electron over a long distance. Thus, to achieve this goal in more efficient and predictable way, I developed a novel design of dinuclear Ru(II) complex having phenazine and diimide units in the bridging ligand as well as one of mononuclear Ru(II) complex having phenazine and anthraquinone units prepared from the building block of the photosensitizing unit [Ru(bpy)₂(dppb)]²⁺ (dppb: dipyrido[3,2-a:2',3'-c]phenazine-benzoyl group). To prepare the rigid and long ranged Ru(II) polypyridyl systems, the imine bond and dppb unit were applied in the Ru(II) polypyridyl systems such as [RuIQ]²⁺ and [Ru2ID]⁴⁺. In particular, the rigid dinuclear Ru(II) polypyridyl complex [Ru2ID]⁴⁺ was easily prepared as the moderate yield (56%) by one-pot synthesis of 2 mol [Ru(bpy)₂(dppb)]²⁺ and 1 mol diimide unit, and the rigid mononuclear Ru(II) polypyridyl complex [RuIQ]²⁺ was also obtained as the moderate yield (55%) through the imine reaction of [Ru(bpy)₂(dppb)]²⁺ and 2-aminoanthraquinone. Every obtained Ru(II) polypyridyl complex was purified by Sephadex LH-20 column following to reprecipitation by addition of aqueous NH₄PF₆, and was easily characterized by IR (imine bond peak), ¹H-NMR and conductivity. The photophysical and redox studies of these Ru(II) complexes will be compared to those of the mononuclear and dinuclear Ru(II) complexes connected to amide bond in the poster section. In addition, I will discuss on the structural studies of the conjugation composed of imine bond by comparison to amide bond in the Ru(II) complex. As a result, [Ru(bpy)₂(dppb)]²⁺ and [Ru(bpy)₂(dppz-NH₂)]²⁺ complexes are a useful building block for constructing efficient photoinduced electron or energy transfer systems. References 1. (a) Choi, C.-S.; Rapid Commun.

Photosci. 2014, 3, 42. (b) Campagna, S.; Serroni, S.; Bodige S.; MacDonnell, F. M. Inorg. Chem. 1999, 38, 692.



Poster Presentation : **MAT.P-481**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Affinity-based Purification of Biopharmaceuticals Using Synthetic Binding Pairs

An Jaeyeon, Junghyun Kim¹, Kyeng Min Park^{1,*}, Kimoon Kim^{*}

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

¹Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Biopharmaceuticals including monoclonal antibodies (mAb) and cytokines have occupied a major class of pharmaceuticals because of their remarkable efficacy compared to chemical drugs. Genetic engineering significantly contributed to high-level expression of therapeutic proteins in mammalian cells and bacteria for the mass production. However, multi-step purification through various chromatographies, mostly due to inefficient isolation of proteins of interest, reduces the efficiency of biomanufacturing. Although protein A-based affinity chromatography has been used for mAb purification, additional chromatographies are typically required for removal of undesired proteins having similar structural properties with the target mAb. In addition, this affinity chromatography cannot be used for other proteins including cytokines which do not have Fc region of immunoglobulins for protein A interaction. Here we report an efficient affinity-based purification method using synthetic binding pairs. The interaction between the binding pair is not affected by biomolecules such as proteins with sufficient enough binding affinity. Thus, this synthetic binding pair system can be a good alternative for purification of therapeutic proteins.

Poster Presentation : **MAT.P-482**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Effect of Styrene-PVP Interaction on the Properties of Silicone Hydrogel Lens

Min-Jae Lee, A-Young Sung*

Department of Optometry, Daegu Catholic University, Korea

This research was carried out in order to analyze the effect of Styrene-PVP interaction on the properties of silicone hydrogel lens. Styrene group and PVP (Polyvinylpyrrolidone) were used as additives for the basic combination containing silicone monomer, TSMa (trimethylsilyl methacrylate) and DMA (n,n-dimethylacrylamide) added to the mix at ratios of 1~10%. The silicone hydrogel lens was produced by a cast-mold method. The polymerized lens sample was hydrated in a 0.9% saline for 24 hours before the optical and physical characteristics of the lens were measured. Measurement of the physical characteristics of the produced material showed that the refractive index is 1.3682~1.4321, water content 77.11~45.73%, visible light transmittance 95.14~88.20%, and tensile strength 0.0652~0.3113kgf. The results showed the decrease of refractive index as the ratio of additives and the water content also decreased. The result of the stabilization test of polymerization showed increase of extractables as the ratio of additives, but the difference was not significant in all the samples, so it can be judged that the stabilization of the polymer was maintained. Therefore, the interaction of styrene and PVP should be in consideration of the effect on the physical properties of silicone hydrogel lens.

Poster Presentation : **MAT.P-483**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Characteristics of Hydrogel Lenses Containing Nanoparticles of Cerium Oxide and Cerium Iron Hydroxide with 4-Chlorostyrene

Su-mi Shin, Jonghwan Do, A-Young Sung*

Department of Optometry, Daegu Catholic University, Korea

The physical properties of hydrogel lenses made of cerium oxide and cerium iron hydroxide nanoparticles containing 4-chlorostyrene as an additive were compared and analyzed. Cerium oxide and cerium iron hydroxide were used to copolymerize with the basic monomer HEMA (2-hydroxyethyl methacrylate), 4-chlorostyrene, N-vinyl-2-pyrrolidone (NVP), 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. 4-Chlorostyrene did not show any significant difference in spectral transmittance, and UV rays were blocked by the effect of cerium oxide and cerium iron hydroxide. As the amount of 4-chlorostyrene, the water contents of cerium oxide group and cerium iron hydroxide group were in the range of 41.72 ~ 24.49% and 41.21 ~ 26.66%, respectively. The breaking strengths were in the range of 0.18343 ~ 2.00092kgf and 0.13311 ~ 1.67409kgf, respectively. In particular, the contact angle and breaking strength of cerium oxide group increased rapidly from 3% content of 4-chlorostyrene and from 5% content of 4-chlorostyrene to cerium iron hydroxide group. 4-Chlorostyrene is an excellent hydrogel lens material that decreases water content, and increases breaking strength without affecting the spectral transmittance.

Poster Presentation : **MAT.P-484**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Enhanced photodegradation of Indigo Carmine using ZnO-Bi₂O₃- Graphitic carbon nitride/H₂O₂ system

Huy B.t., Yong-ill Lee*

Department of Chemistry, Changwon National University, Korea

ZnO-Bi₂O₃-Graphitic Carbon Nitride/H₂O₂ system degraded 93% of Indigo Carmine in aqueous solution (50 mg/L) under visible irradiation in 180 min. The heterostructural material of ZnO-Bi₂O₃-Graphitic Carbon Nitride was prepared using co-precipitate method at 80 °C. The mechanism of photocatalytic degradation of Indigo carmine shows the responsible species for the degradation of Indigo carmine is the hydroxyl radicals which were generated from the reaction of e^- and h^+ with H₂O₂. Besides, the kinetic of the photocatalytic process was detailed. The prepared catalyst displayed excellent stability during four cycles. These results demonstrate that the ZnO-Bi₂O₃- Graphitic Carbon Nitride/H₂O₂ system may become a promising technique for removing harmful organic dyes through advanced oxidation processes. Keywords: Photocatalyst, Indigo Carmine, degradation, heterostructure., mineralization.

Poster Presentation : **MAT.P-485**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Eu-doped Bi₂WO₆ for the photodegradation of 2,4,5-Trichlorophenoxyacetic acid.

Seong-Soo Lee, Huy B.t.¹, Yong-ill Lee^{1,*}

Changwon National University, Korea

¹Department of Chemistry, Changwon National University, Korea

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-486**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of ternary Pt-Ni-Cu octahedra for electrocatalytic methanol oxidation reaction

Youngmin Hong, Sang-II Choi*

Department of Chemistry, Kyungpook National University, Korea

A direct methanol fuel cell (DMFC) has been considered as a promising energy system for the application of portable electronics and aerial vehicles such as drones. Nanoscale Pt based materials have been extensively studied in recent years owing to their superior activity for the methanol oxidation reaction (MOR). Among Pt based materials, Pt alloying with other transition metals cheaper than Pt such as Co and Ni was considered promising materials. Here we present the synthesis of 9 nm ternary Pt-Ni-Cu octahedra with the use of oleylamine and oleic acid as surfactants and CO gas as the capping agent for Pt{111} facets. We show that the electrocatalytic activity and stability of Pt-Ni-Cu ternary alloy octahedra toward the MOR were improved compared to those of the commercial Pt/C catalysts, mainly due to the enhanced CO tolerance by the existence of Cu and Ni.

Poster Presentation : **MAT.P-487**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Surface Elemental Distribution Impact of Pt-Pb Hexagonal Nanoplates as Electrocatalysts toward Methanol Oxidation Reaction

Hee Jin Kim, Sang-II Choi*

Department of Chemistry, Kyungpook National University, Korea

The development of bimetallic Pt-based catalysts have been studied to improve the performance of direct methanol fuel cells because CO, a poisoning intermediate, reduces the catalytic activity of pure Pt catalysts. Herein, we synthesized Pt-Pb hexagonal nanoplates as electrocatalysts towards methanol oxidation reaction (MOR) and further control the Pt and Pb distributions on the surface of nanoplates through acetic acid (HAc) treatment. Consequently, we obtained Pt-Pb nanoplates and HAc-treated Pt-Pb nanoplate with homogeneous and heterogeneous distributions of Pt-Pb alloy surfaces, respectively. Pt-Pb nanoplates were exhibited enhanced electrocatalytic properties for MOR relative to HAc-treated Pt-Pb nanoplates, due to enhanced CO tolerant by modifying the electronic structure of Pt under the influence of oxophilic Pb.

Poster Presentation : **MAT.P-488**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Study of electronic structures and cation disorder behavior of lithium transition metal oxides (LMO, M = Co and Ni) with various lithium composition from first principles calculation

Hyosik Kang, Sanghun Lee*

Nanochemistry, Gachon University Global Campus, Korea

Lithium ion battery (LIB) has been the most popular energy storage device for portable electronics due to its high energy and power density. Among many materials for the cathode, the layer-structured LiCoO₂ has been most widely employed for LIB since its first commercialization by SONY. Thus, a lot of experimental as well as calculational investigations have been performed to characterize properties of LiCoO₂ for decades. Meanwhile, to overcome several drawbacks of LiCoO₂, such as, environmental risk and high cost, many efforts to replace Co with alternative transition metals, for example, Ni, have been made. The main problem of LiNiO₂ is the formation of nonstoichiometric lithium nickel oxide and the high level of “cation disorder” or “cation mixing” behavior of Li and Ni ions. In this work, the electronic structures of lithium transition metal oxides (LiCoO₂, Li_{0.5}CoO₂, CoO₂, LiNiO₂, Li_{0.5}NiO₂, and NiO₂) and the cation disorder in Li_xMO₂ (x = 0.98, 0.92, 0.85) are investigated using the density functional theory (DFT) calculations. For a reasonable estimation of the band structure and the density of state (DOS) of LiCoO₂, we managed to obtain Hubbard U for Co. The calculated electronic structures of fully lithiated systems are in good agreement with the previous studies and accord with predictions. However, in the cases of half-lithiated ones, the band structure and DOS are out of predictions, which, we believe, comes from its asymmetric geometry around oxygen atoms. In addition, the energy barrier for cation disorder in LiNiO₂ is much lower than that in LiCoO₂, which is consistent with the experimental observation.

Poster Presentation : **MAT.P-489**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

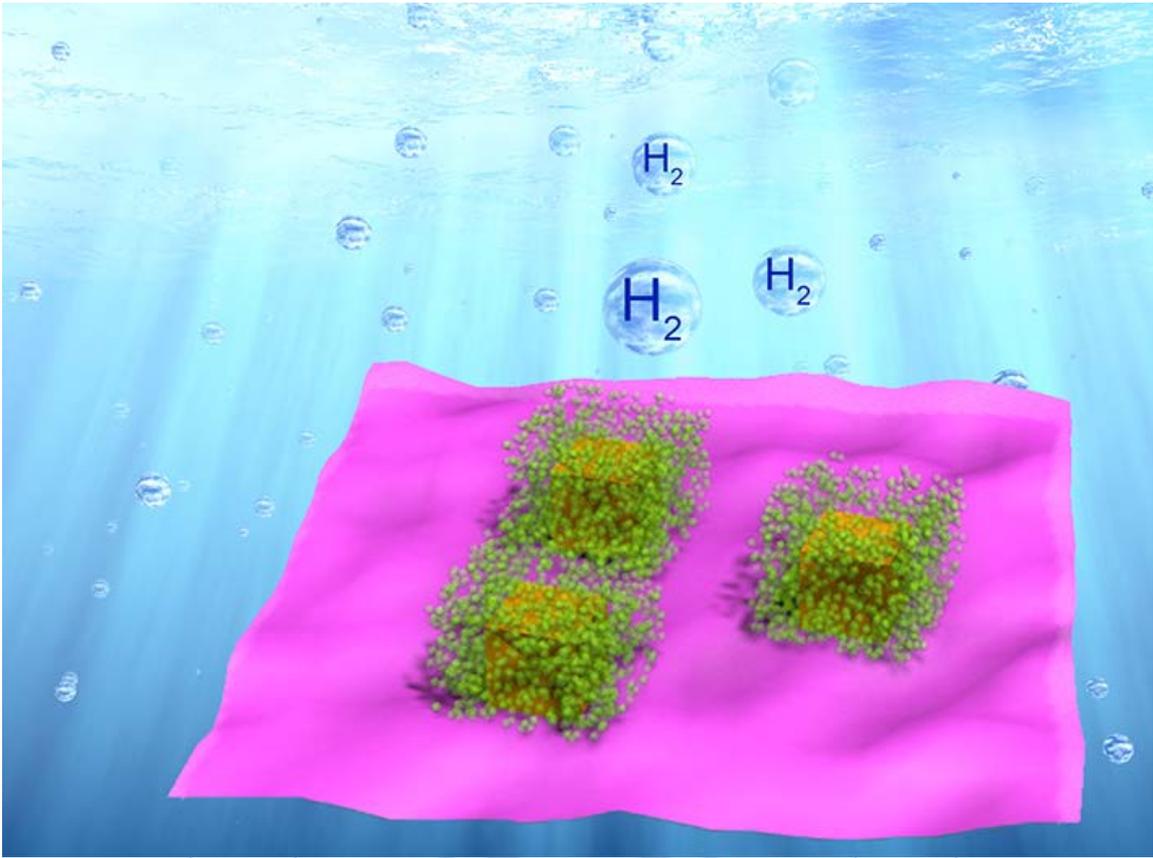
Intimately-coupled MoS₂-Au-CdS ternary hybrids for efficient visible-light photocatalytic hydrogen evolution

Dae Han Wi, Jong Wook Hong¹, Sang Woo Han*

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

¹*Chemistry, University of Ulsan, Korea*

Solar-driven production of chemical fuels through photocatalysis holds great promise for addressing the ever-increasing energy and environmental issues. However, its practical application is limited due to low light harvesting efficiency, fast charge recombination, and low stability of current photocatalysts. Here, we introduce a high-performance solar energy conversion platform constructed by the intimate coupling of two different complementary semiconductors (MoS₂ and CdS) and morphology-controlled plasmonic metal nanocrystals (concave cubic Au nanocrystals) in a controlled manner. The sequential Au nanocrystal anchoring and CdS growth on two-dimensional exfoliated MoS₂ nanosheets successfully yielded intimately coupled plasmonic metal–semiconductor ternary hybrids. The prepared hybrid photocatalysts exhibited superb hydrogen evolution capability under visible-light irradiation, which can be attributed to the synergistic integration of the advantages of semiconductor–semiconductor coupling, such as the broadening of light absorption and the retardation of charge recombination, and plasmon energy transfer from Au nanocrystals to semiconductors via the hot electron transfer mechanism.



Poster Presentation : **MAT.P-490**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and Characterization of Colloidal Gallium Nitride Quantum Dots and Impurity Doping for Blue Emission

Yun Chang Choi, Chiho Lee, Juhee Son¹, Sungnam Park, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

¹*Chemistry, Korea University, Korea*

Gallium nitride (GaN) has been of interest due to its enormous potentials for optoelectronic devices. However, it is very interesting that no proper bottom-up chemical synthesis method for GaN quantum dot has been proposed. Here, we first present a new synthetic method for GaN colloidal quantum dots based on the hot-injection technique. Strikingly, it was possible to demonstrate the change in the emission energy of GaN CQDs by adjusting their reaction condition, which directly shows the existence of quantum confinement effects in colloidal GaN CQDs. Furthermore, the ultraviolet emission of colloidal GaN CQDs has been lowered to the blue region by introducing Zn metal impurities, which has never been observed in the colloidal nitride nanocrystal system. The origin of blue emission was studied with time-resolved photoluminescence (TRPL). This GaN CQD study would provide a new perspective on III-V colloidal nanocrystal system, and basis for optoelectronic applications of colloidal quantum dots.

Poster Presentation : **MAT.P-491**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

One-pot synthesis of dendritic PtNi nanocrystals on CeO₂ nanosheets as supporting materials with high electrocatalytic performances toward methanol electrooxidation and oxygen electroreduction.

Yongmin Kwon, Sang Woo Han^{1,*}

Korea Advanced Institute of Science and Technology, Korea

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

The development of supporting material for electrocatalysis with additional promoting effects is essential for designing innovative fuel cell catalysts. Due to its high density of oxygen vacancies, CeO₂ enables to suppress the poisoning of active sites in Pt-based catalysts and is considered to be one of the best candidates for supporting materials. Here, we report a facile one-pot synthesis strategy for PtNi/CeO₂ hybrid nanostructures with well-defined and dispersed dendritic PtNi nanocrystals on CeO₂ nanosheets as supporting material. The prepared PtNi/CeO₂ nanostructures exhibited outstanding electrocatalytic properties toward both methanol electro-oxidation and oxygen electro-reduction owing to high oxygen storage capacity of CeO₂ support and arbitrated electronic structure. CeO₂ nanosheets, the reinforced supporting material than other carbon based, enhanced not only the activity but also durability of the catalysts.

Poster Presentation : **MAT.P-492**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

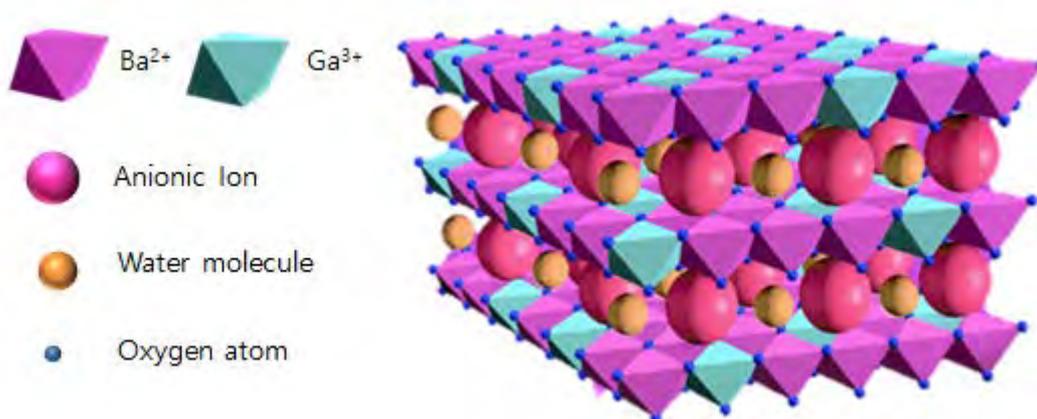
Synthesis of BaGa-Layered double hydroxide for multimodal contrast agent application

So Yeon Yun, Jin Kuen Park^{1,*}

Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

We synthesized Layered double hydroxide (LDH) using barium and Gallium for achieving multimodal contrast agent. It was intended to develop multi-imaging active bio-ceramic based intergrated materials that can be activated by response to in vivo environments and which have contrast medium functions in more than one medical imaging device. Previously, no paper had synthesized LDH with Barium and Gallium. Barium species have a characteristic as computed tomography (CT) and magnetic resonance imaging (MRI) contrast properties and radioisotope Gallium is available as positron emission tomography (PET) contrast function. These two materials were synthesized to synthesize multiple contrast material with both advantages. Powder X-ray diffraction (PXRD) patterns revealed a typical characteristic of LDH, and it was verified that size and morphology by scanning electron microscopy (SEM).



Poster Presentation : **MAT.P-493**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Magnetic field-assisted self-assembled plasmonic chiral film with tunable optical activity

Ki-Jae Jeong, Dong-kyu Lee, Van Tan Tran¹, Caifeng Wang, Jaebeom Lee^{1,*}

Department of Cogno-Mechatronics Engineering, Pusan National University, Korea

¹*Chemistry, Chungnam National University, Korea*

Helix is representative structures which shows optical activity. In nature, helical structures exist everywhere. From the molecular level for example biological molecules such as DNA, amino acid to cosmic phenomenon, planetary movement, gravitational wave, we can easily find the chiral and helical structures and vortex movements, and circularly polarized waves. The origin of chirality is coming from the structural asymmetry. Chiral structures such as helix have no any symmetric point, line, and plane. So it cannot be overlapped with its symmetric images. This figures can give different interactions with right- and left-handed circular polarized light. Here, we fabricated nature-inspired helix-mimetic optical activity modulator with self-assembled magnetoplasmonic nanochains. In the polymer gel and solution, we can assemble magnetic nanochain by external magnetic field. In addition, we can control its structures by physical force and magnetic field arrangement. As a results, circular dichroism signal intensities and sign can be changed.

Poster Presentation : **MAT.P-494**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Visible light photocatalytic property Of M/ATO/TiO₂ (M=Au, Ag and Pt)

Hye Jin Kang, Wan-In Lee*

Department of Chemistry, Inha University, Korea

TiO₂ has been known to be the most efficient photocatalyst among various semiconductors. However, TiO₂ with wide band gap can utilize only the photons in the UV region. Hence, in order to be able to utilize the major portion of the solar spectrum, designing novel photocatalysts that can utilize visible light is prerequisite in enhancing photocatalytic efficiency and extending the range of applications. A promising approach is the formation of a heterojunction structure between the sensitizer and the main photocatalyst. In the present work, we doped Sb ions into SnO₂ to form antimony-doped tin oxide (ATO), which absorbs a considerable portion of visible-light with its deep-blue color. We found that ATO is an effective sensitizer for use with TiO₂ in forming the heterojunction structure with high visible light photocatalytic activity. The VB of the ATO is located lower than that of TiO₂. Under visible light irradiation, the electrons in the VB of the ATO are excited to its CB. Thereby, the VB of the ATO is rendered partially vacant, and the electrons in the VB of TiO₂ can be transferred to that of ATO. As a result, holes are generated in the VB of TiO₂, initiating in turn various oxidation reactions. For further enhancement of visible-light catalytic efficiency, we selectively deposited Au, Ag and Pt on the ATO surface using the photodeposition method with visible light. The deposition of noble metal on the ATO surface significantly increases the photocatalytic efficiency. Higher catalytic efficiency is due to the retardation of charge recombination for ATO NPs, leading to expedition of hole-transport from VB of ATO to that of TiO₂.

Poster Presentation : **MAT.P-495**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Simulational study for forming mechanism of the pores in FeOOH nanorod

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¹*Pusan National University, Korea*

²*Chemistry, Chungnam National University, Korea*

One-dimensional (1D) mesoporous magnetite nanorods are attractive owing to porous morphology and anisotropic magnetic properties, in particular, in the application of electrochemistry and energy storage. Here, magnetic nanorods containing ordered mesocages are synthesized. Based on Cahn-Hilliard equation, by using phase-field simulation with finite element method, a process for the formation of the mesocage nanostructures was proposed. Mechanism of pore coarsening caused by dissolution and recrystallization process on the interface of the aqueous solution state of pore and solid state of FeOOH crystal was explained. Through the Arrhenius equation, thermodynamic energy that affects the dissolution and re-crystallization on the specific thermodynamic condition, was calculated. Moreover, it has been shown through the simulation that thermodynamic energy of the solid-liquid interface inside the nanostructure determines the formation process and the final morphology of the pores. Synthesized ordered mesocage nanorods are promising for the fabrication of new electroactive functional material for next-generation energy-related applications as well as novel catalysts.

Poster Presentation : **MAT.P-496**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

PdAg@Pd Core–Shell Catalysts for Efficient Hydrogen Production from Formic Acid Decomposition

Bon Seung Goo, Sang Woo Han*

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

To develop high-performance bimetallic catalysts, fine control over both the ligand and strain effects of secondary elements on the catalytic function of primary elements is crucial. Here we introduce an approach to produce Pd–Ag bimetallic core–shell nanocatalysts with synergistic regulation of the ligand and strain effects of Ag. Through precise core–shell engineering, (PdAg alloy core)@(ultrathin Pd shell) nanocrystals with controlled core compositions and shell thicknesses in addition to a well-defined octahedral morphology could be realized. The prepared octahedral PdAg@Pd core–shell nanocrystals exhibited pronounced catalytic performance toward hydrogen production from formic acid decomposition. The maximum catalytic activity was achieved with PdAg@Pd nanocrystals consisting of PdAg alloy cores with an average Pd/Ag atomic ratio of 3.5:1 and 1.1 atomic layer of Pd shells, which showed a record high turnover frequency of 21 500 h⁻¹ at 50 °C. This catalytic function could be attributed to the optimized combination of the electronic promotion and lattice strain effects of Ag on Pd. We envision that the present work can provide a rational guideline for the design of improved catalysts for various important chemical and electrochemical reactions.

Poster Presentation : **MAT.P-497**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

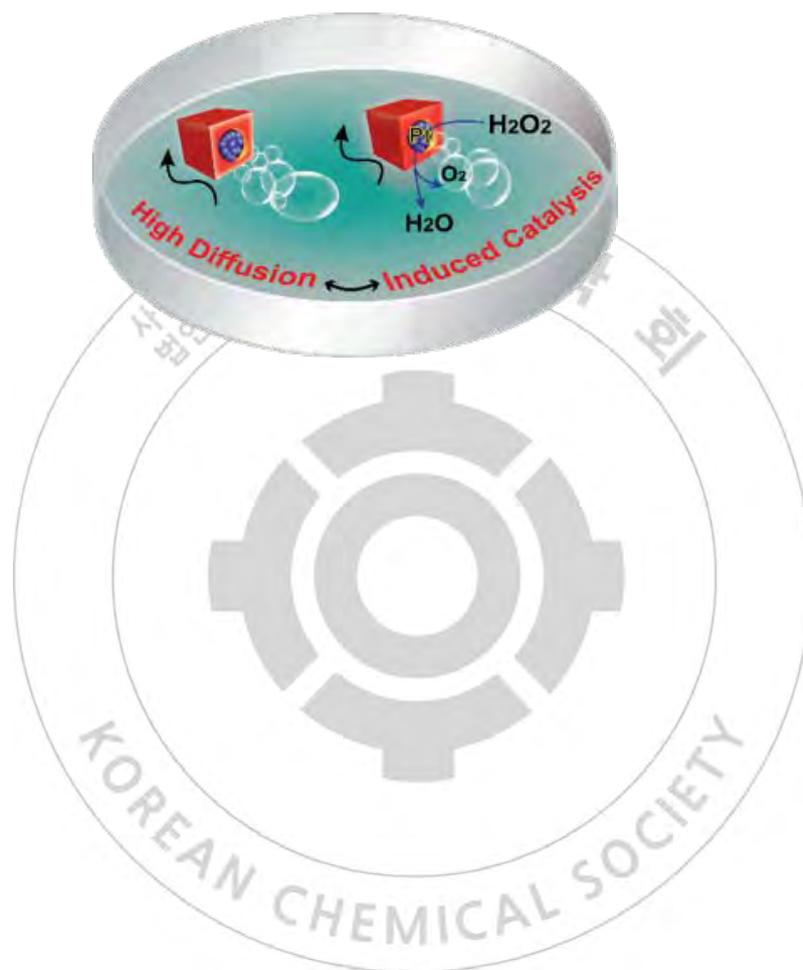
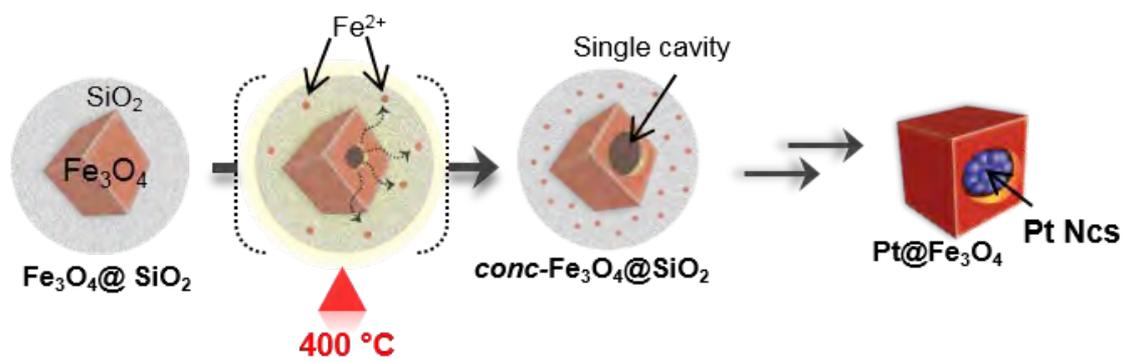
Monofacet-Selective Cavitation within Solid-State Silica-Nanoconfinement towards Janus Iron Oxide Nanocube

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

In spite of the tremendous application potential, the synthesis of the 3-dimensional nanocrystals with anisotropic high-energy negative surface-curvature is still elusive. The demand of such concave surface-NCs (CS-NCs) stems from their diverse applications in catalysis, plasmonics, medicine and their facile post-synthetic engineering to create programmable compositions and geometrical arrangements integrating different functionalities in single nanostructure. Here, a highly selective solid-state nanocrystal conversion strategy is developed towards concave iron oxide (Fe₃O₄) nanocube with an open-mouthed cavity engraved exclusively on a single face. The strategy is based on a novel heat-induced nanospace-confined domino-type migration of Fe²⁺ ions from the SiO₂-Fe₃O₄ interface towards the surrounding silica shell and concomitant self-limiting nanoscale phase-transition to the Fe-silicate form. Owing to the unique nanoscale architecture and distinguished chemical nature of concave cavity in the transformed iron oxide nanocube (conc-Fe₃O₄), catalytic Pt-grains were exclusively and controllably functionalized within the cavity, resulting Janus Fe₃O₄@Pt structures which can act as catalytically self-propelled highly diffusive nanoswimmers for the efficient removal of common pollutant-dyes from water. Reference: J. Am. Chem. Soc. 2018, 140, 15176-15180.



Poster Presentation : **MAT.P-498**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Hydrothermal Synthesis of CuMO_2 (M= Ga, Cr) for Inorganic Hole Conductor

Mintai Jung, Wan-In Lee*

Department of Chemistry, Inha University, Korea

Several delafossite metal oxides have been known to be a potential p-type transparent conducting oxide (TCO). The chemical formula of delafossite metal oxide is ABO_2 , where A=Pt, Pd, Cu, Ag, and B=Al, Ga, In, Sc, etc. It is a kind of layered structure consisting of linearly coordinated O-A-O layer and edge-sharing octahedral BO_6 layer. With its excellent p-type conductivity and high optical transparency, delafossite structures have been proposed as functional materials for various electronic applications, including transparent p-n junction devices, photo- and electrochemical catalysis such as water splitting and reduction of CO_2 , and hole conductor material for solar cells. For the application of delafossite materials as hole conductor, it is necessary to obtain ultrafine nanoparticles (NPs) with high monodispersity, because high quality thin films cannot be achieved from large particles. In this work, we synthesized CuCrO_2 and CuGaO_2 NPs by hydrothermal method with soluble metal nitrate salts as precursors. $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$, $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{Ga}(\text{NO}_3)_3 \cdot x\text{H}_2\text{O}$ were dissolved in deionized water, followed by NaOH as a mineralizer. The corresponding solutions were transferred into a Teflon-lined autoclaves, and then kept at 240°C for 48h. With the presence of several surfactants and mild reducing agents, CuGaO_2 hexagonal nanodiscs with diameters in the range of 20~50 nm were successfully obtained. We also obtained highly uniform CuCrO_2 hexagonal nanodiscs with diameter of 9 nm. The prepared CuCrO_2 and CuGaO_2 nanodiscs were applied as hole transporting layer of perovskite solar cells.

Poster Presentation : **MAT.P-499**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

New Lithium-ion Conducting Framework Oxide, LiTa_2PO_8

Doe-hee Park, Jaegyeom Kim, Gunwoo Yoo, Seung-Joo Kim*

Department of Energy System, Ajou University, Korea

Inorganic solid lithium-ion conductors can be substituted for existing organic liquid electrolytes to solve safety issues for lithium-ion battery. For this reason, many efforts have been devoted to explore new solid-state lithium-ion conductors having high lithium-ion conductivity and chemical/electrochemical stability. Here, we report a fast lithium-ion conducting oxide, LiTa_2PO_8 for the first time that has a novel three-dimensional (3D) framework structure. The complementary use of synchrotron X-ray and neutron diffraction revealed that LiTa_2PO_8 crystallized into a monoclinic system (space group $C2/c$) with lattice parameters $a \approx 9.716 \text{ \AA}$, $b \approx 11.536 \text{ \AA}$, $c \approx 10.697 \text{ \AA}$, and $\beta = 90.04^\circ$. In this structure, the TaO_6 octahedra and PO_4 tetrahedra are connected via corner-sharing to form an unprecedented anionic framework, $[(\text{TaO}_{6/2})_2(\text{PO}_{4/2})]^-$, providing a 3D pathway for lithium-ion conduction. The sintered LiTa_2PO_8 pellets exhibited excellent lithium-ion conductivities: bulk conductivity of $1.6 \times 10^{-3} \text{ S cm}^{-1}$ and total conductivity of $2.5 \times 10^{-4} \text{ S cm}^{-1}$ at 25°C .

Poster Presentation : **MAT.P-500**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The phase transition and thermochromic characteristics in W- and Nb-doped VO₂(M) nanocrystallites and their thin films

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Department of Chemistry, Pukyong National University, Korea

¹*Research & development center, Adchro Inc., Korea*

Switchable chromic materials belong to the most important category of advanced functional materials. There are three important types of switchable chromic materials: photochromic, thermochromic and electrochromic materials. All these materials can modulate the optical transmittance by either light, heat or electricity. Thermochromic material among them is a kind of self-controlling by surrounding temperature. Thus the application of thermochromic materials to energy-saving smart window is one of hot topics. VO₂(M) that shows a reversible crystal phase transition from monoclinic to rutile at higher temperature changes electrical conductivity from semiconductor to metal concomitantly with phase transition. This electrical conductivity change modulates near infrared (N-IR) transmittance. Therefore VO₂(M) has been widely recognized as a good candidate for smart window application. Since the transition temperature (T_c) of pure VO₂(M) is too high for practical application, the lowering T_c is a key factor for successful application. Widely studied method of lowering T_c is doping of some other transition metal cations into VO₂(M). Although the doping of a certain cation such as W could reduce T_c very effectively but it also seriously deteriorated the transition sharpness and NIR switching efficiency dramatically decreased. Maintaining the transition sharpness is also important as well as lowering T_c. In this study we have prepared W- and Nb-doped VO₂(M) nanocrystallites with various amounts of dopants by hydrothermal and post thermal transformation method and closely investigated the doping effect on the transition characteristics. We also prepared the thin films of these doped VO₂(M) on PET substrate by a wet-coating method from their solvent-dispersed coating solutions. The relationship between N-IR transmittance changes of these doped thin films and their crystal phase transition were investigated.

Poster Presentation : **MAT.P-501**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Impact of large mesopores of carbon electrodes on electrochemical performance of EDLCs

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

Electrochemical double layer capacitors (EDLCs) store electrochemical energy via adsorbing electrolyte ions on the electrode surface. High specific surface area (SSA) and good electric conductivity of carbonaceous materials have been mainly considered as utmost factors governing electrochemical performance of EDLCs. In this regard, numerous attempts have focused on increasing SSA via developing micropores and mesopores of carbons; on the other hands, large mesopores have been less focused. In this poster, we present how large mesopores of carbonaceous materials impact on electrochemical performance of EDLCs in a full-cell configuration 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 (10-40 nm) of 3DOMCs with similar surface areas were investigated and the correlation between the size of mesopores and capacitances will be presented.

Poster Presentation : **MAT.P-502**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Electron transporting materials for blue phosphorescent organic light-emitting diodes using triaryl boron derivatives

Sunhee Lee, Won-Sik Han^{*}, Sooyeon Kim¹

Department of Chemistry, Seoul Women's University, Korea

¹*Department of Chemistry, Seoul women's university, Korea*

Two duryl borane derivatives, tris(2,3,5,6-tetramethyl-4-(pyridin-3-yl)phenyl)borane (TDPB) and tris(2,3,5,6-tetramethyl-4'-(pyridin-3-yl)biphenyl-4-yl)borane (TDPPB), which contain heteroaromatic pyridine rings at peripheral positions were synthesized to investigate the effects of bridging phenyl group on their thermal, photophysical, and electrochemical properties. Upon adding a phenyl unit between duryl and pyridine units, TDPPB showed slightly higher thermal stability ($T_d = 446$ °C and $T_g = 166$ °C) than TDPB ($T_d = 439$ °C and $T_g = 142$ °C). Both TDPB and TDPPB have deep highest occupied molecular orbital levels to block the holes/excitons and appropriate lowest unoccupied molecular orbital levels for smooth electron injection. Notably, TDPB and TDPPB exhibited relatively high triplet energies of 2.84 eV and 2.69 eV, respectively. Thus, the triplet energy level of TDPB is sufficient for use in bis[2-(4,6-difluorophenyl)pyridinato-C2,N](picolinato)iridium(III) (FIrpic) based blue phosphorescent organic light-emitting diodes (PHOLEDs) as an electron transport material. Accordingly, TDPB was used as an electron transport material in FIrpic-based blue PHOLEDs and the optimized device showed high external quantum efficiency of up to 18.8%.

Poster Presentation : **MAT.P-503**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Size and shape control of TiO₂ nanoparticles

Youngin Jeon, Wan-In Lee^{1,*}

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¹*Department of Chemistry, Inha University, Korea*

TiO₂ nanoparticles (NPs), widely used as photocatalysts and employed as electron transport layer (ETL) of several solar cells, were prepared by solvothermal reaction of Ti-alkoxide in ethanol/water mixture. The size of TiO₂ NP is an important factor in constructing the ETL architectures suitable for inorganic hybrid solar cells. Surface morphology of TiO₂ NPs is considered to be another important factor for the formation of ETLs, because the connectivity between NPs in the ETL is strongly dependent on their surface structures. In principle, size of TiO₂ NPs can be controlled by changing the ratio of ethanol/water, as the hydrolysis reaction of Ti-alkoxide is influenced by water content. Herein, we varied ethanol/water ratios to 45:55, 35:65, 25:75, 15:85, 5:95 and 0:100, while an alkylamine was used as basic catalyst. As the component of ethanol increases, the size of TiO₂ NPs decreases and their shapes change to spherical. When the ethanol component is high, sol-gel reaction becomes slow, and the anisotropic growth to a certain direction is suppressed. Thus, the initially formed TiO₂ nuclei undergo isotropic growth and form polygon or spherical structures. Contrarily, as the water component increases, the size of TiO₂ NPs increases and their morphologies become rod-like structures. When the water content is high, sol-gel reaction of Ti-precursor is accelerated, inducing fast growth of NPs. As a result, crystal growth toward the (001) direction is accelerated, and the prepared TiO₂ NPs become rod-like shape. Various TiO₂ NPs were employed as ETLs of perovskite solar cell devices, and we found that the NPs with spherical shape provide the highest photovoltaic performance.

Poster Presentation : **MAT.P-504**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Low-cost Synthesis of Mesoporous Hollow Silica Spheres for CO₂ Capture

Suguan Jang, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

In this study, we synthesized mesoporous hollow silica spheres (MHSS) using two types of precursors to synthesize low-cost CO₂ capture support. One was MHSS-SS using sodium silicate(SS) as a low-cost precursor and the other was MHSS-TS using TetraethylOrthosilicate (TEOS) as a precursor. MHSS materials were synthesized from core-shell structured polystyrene (PS) core with mesoporous silica shell. Two types of MHSS were synthesized and modified by wet impregnation with tetraethylenepentamine (TEPA) as solid adsorbents. The synthesized materials were characterized various method such as TEM, XRD, N₂ adsorption/desorption, FT-IR, and TGA and their CO₂ capture capacity was tested. The MHSS-SS showed that the pore size of 3.80 nm, BET surface area of 1300 m²/g, pore volume of 0.40 cc/g, which was not significantly different from MHSS-TS. In addition, we compared the CO₂ capture performance with the use of two types of silica materials as supports. The low-cost silica precursor CO₂ adsorption performance was not significantly different from the expensive silica precursor.

Poster Presentation : **MAT.P-505**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Rational design of carbazole-based donor–acceptor dyad system for thermally activated delayed fluorescent material

Keumhee Lee, Taebin Cha*, Won-Sik Han*

Department of Chemistry, Seoul Women's University, Korea

A series of donor–acceptor compounds has been designed and prepared. Photophysical-and electrochemical properties of prepared compounds were investigated systematically. Carbazole is adopted as a donor (D) fragment, while benzophenone is selected as acceptor fragment. Depending on the bulkiness of bridge unit, two compounds showed significantly different characters. Namely, when the donor and acceptor was connected by phenyl ring, electronic communication between donor and acceptor was engaged and showed typical charge transfer (CT) character in photoluminescence spectrum. On the other hand, when two units were connected by bulky unit, tetramethyl phenyl ring, electronic communications between two units were completely blocked. This phenomenon was fully supported by using density functional theory and time dependent density functional theory. Accordingly, their triplet energy levels were tuned easily, thus the singlet–triplet energy gaps (ΔE_{ST}) can be controlled by simple modification of molecular structure. Our design strategy might provide more chances to challenge the rational design of novel and high-performance TADF-based organic light emitting diodes.

Poster Presentation : **MAT.P-506**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Hard-templating synthesis of ordered mesoporous carbon without acid-catalyst impregnation

Hakju Lee, Kyoungsoo Kim*

Department of chemistry, Chonbuk National University, Korea

In the hard-templating synthesis for ordered mesoporous carbon, acid catalysts are normally used to polymerize organic carbon sources within the template pores, and hence to increase the amount of carbon converted from the organic sources. However, the synthesis involving the acid-catalytic polymerization requires several time and cost consuming steps because the acid catalyst should be impregnated with carbon sources into the template pores or incorporated onto the pores as a solid acid. In the present work, we synthesized ordered mesoporous carbon CMK-3 through the carefully controlled polymerization process, excluding use of acid catalyst. Furfuryl alcohol was used as a carbon source, and their polymerization proceeded by thermal heating at various temperatures and ramping rates. The resultant carbon structures were characterized by X-ray diffraction, N₂ adsorption/desorption analysis and electron microscopy. The results indicated that the mesoporous carbon having high surface, pore volume, and pore regularity could be obtained without acid catalyst. The well-defined structure is comparable to those of carbon synthesized after acid-site incorporation onto the template pores. Notably, the carbon synthesized under the acid-free condition exhibited high oxygen contents as compared to the carbon synthesized conventionally. The oxygen content was increased with the polymerization temperature. Furthermore, we analyzed electrochemical properties of the carbon products. The carbon synthesized with higher polymerization temperature exhibited higher electrochemical capacity. The result can be attributed to increase of oxygen content in the carbon framework according to the polymerization temperature.

Poster Presentation : **MAT.P-507**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Zeolite templated micropore 3D graphene carbon synthesis for lithium ion capacitor application

JinJu Han, Hakju Lee, Kyoungsoo Kim*

Department of chemistry, Chonbuk National University, Korea

A lithium-ion capacitor (LIC) is a hybrid energy storage device that consists of a high-energy lithium-ion battery anode and a high-power electrochemical capacitor cathode. By combination of complementary features of the battery and the capacitor, the LIC can have both high energy and high power density. Various metal oxides, such as TiO_2 , Fe_3O_4 , V_2O_5 and Nb_2O_5 , are widely explored as the anode, but no one except for activated carbons and several nanostructured carbons is actively studied as the cathode. In the present work, we investigated the potential of microporous 3D graphene-like carbons (MGLC), synthesized by hard-templating approach using zeolite template, as a LIC cathode material. The half-cell test showed that the MGLC electrode could work without electrochemical degradation up to the voltage of 4.3 V vs Li/Li^+ . The result indicates strong electrochemical stability of MGLC at high potential voltage, which is a requirement for the cathode application. Taking into account of half-cell results, we assembled the full-cell LIC using MGLC cathode and lithium titanate anode with 2:1 mass ratio of the two electrodes, and measured the capacity in the voltage range from 0 to 2.8 V. The capacitor exhibited a storage capacity of 73.2 F g^{-1} at 0.1 mA cm^{-2} . Notably, the value is 3.3 times larger than the capacity of the device composed of activated carbon and lithium titanate, which results from 3D pore structure and high accessible surface area of MGLC. Furthermore, the capacitance was stable during 30 cycles, indicating strong rigidity of porous carbon frameworks in MGLC.

Poster Presentation : **MAT.P-508**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis and characterization of the homoleptic Ir(III) complex with closed 2-phenylquinoline ligand for red phosphorescent organic light-emitting diodes

SoYoung Kwak, SoHee Lee, Won-Sik Han*

Department of Chemistry, Seoul Women's University, Korea

A new Ir(III) complex, C-PQ were synthesized for red phosphorescent organic light-emitting diodes (PhOLEDs) and its photophysical, electrochemical, and electroluminescent (EL) properties were systematically investigated. For the comparison, its reference complex, O-PQ was also investigated and compared with C-PQ. A comprehensive study of the photophysical properties for these complexes reveals that C-PQ with the rigid structure of the ligand, the radiative rate constant (k_r) is significantly higher than that of reference complex, O-PQ, and contributes substantially to the increase in Φ_{PL} . Experimental and computational evidence clearly supports an enhancement of the metal-to-ligand charge transfer (MLCT) character of the excited state via destabilization of the HOMO, is mainly responsible for the faster radiative rates.

Poster Presentation : **MAT.P-509**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Phase and structure-dependent effects of TiO₂ in application to photocatalytic CO₂ conversion reactions

Dongil Won, Wan-In Lee^{1,*}

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¹*Department of Chemistry, Inha University, Korea*

Various kind of TiO₂ such as commercial P25 TiO₂, [001] phased TiO₂, mesoporous spherical TiO₂ and their disordered structure named as black TiO₂ were synthesized. Pt NPs were then deposited on the prepared TiO₂ by a well-known photodeposition method in order to investigate phase and structure-dependent effects of TiO₂ in the photocatalytic CO₂ conversion reaction. In evolving CH₄ from CO₂ under Xenon lamp (UV-vis light) irradiation, the photocatalytic activities of Pt/P25 TiO₂ are not critically influenced because of their low activated surface structure, whereas using Pt/[001] phased TiO₂, the photocatalytic activities are remarkably increased, clearly indicating that the enhancement of the catalytic activities is caused by exposed surface activation effect of [001] TiO₂. Also, mesoporous spherical TiO₂ showed high photocatalytic activities due to porous structure. Furthermore above TiO₂ catalysts can be further increased in efficiency by inducing defect structure on the TiO₂ surface.

Poster Presentation : **MAT.P-510**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Multifunctional amorphous TaOx layers on photocathodes for photoelectrochemical H₂ production

Sang-Youn Chae, Oh-Shim Joo^{1,*}

Clean energy research center, Korea Institute of Science and Technology, Korea

¹*Korea Institute of Science and Technology, Korea*

Ideal photoelectrodes have high catalytic kinetics and low charge recombination rates to efficient photoelectrochemical reactions. However, most of the semiconductor materials can not satisfy the ideal characters for photoelectrodes. Therefore, several components (e.g., co-catalyst, passive layer, or protection layer, etc.) have usually been applied for one photoelectrode structure. However, the additional interfaces can be recombination sites, and hinder light absorption of the semiconductor. Therefore, we have designed the multifunctional a-TaOx layer minimizing interfaces to improve CuInS₂ photocathodes and simplify the structure of the photoelectrode. We observed the amorphous TaOx was transformed into an active phase during photoelectrochemical reactions, improving the activity of H₂ production. The TaOx multifunctional layer enhanced not only catalytic activity but also charge separation and stability. An a-TaOx/CuInS₂ photocathode shows higher photocurrent compared to Pt/CuInS₂ at -0.3 V vs. RHE applied potential. The charge transportation at the interface of TaOx/CuInS₂ was also investigated by electrochemical impedance spectroscopy.

Poster Presentation : **MAT.P-511**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis Method of Multi-Shell Mesoporous Hollow Silica Nanospheres for CO₂ Adsorption

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Mesoporous Hollow Silica materials have a high specific surface areas and high thermal stability and can be potentially applied in drug delivery, nano catalyst, gas adsorbents. In this study, we synthesized multi-shell mesoporous hollow silica nanospheres(MMS) and prepared CO₂ adsorbents to confirm the ability as gas adsorbents. CO₂ adsorbents were prepared by impregnation methods using tetraethylenepentamine(TEPA) as an amine source. MMS were prepared by sol-gel method using polystyrene as a core material and poly(ethyleneglycol)-block-poly(propyleneglycol)-block-poly(ethyleneglycol)(P123) and cetyltrimethylammonium chloride(CTACl) as dual templates and tetraethylorthosilicate(TEOS) as a precursor. MMS characterized by using FourierTransform-Infrared spectroscopy (FT-IR), N₂-sorption, X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM) and Gas Chromatography (GC) analysis.

Poster Presentation : **MAT.P-512**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Facile Synthesis Method of Fluorine Functionalized Polysilsesquioxanes by Sol-Gel Reaction of Trifluoropropyltrimethoxysilane

Han Jun Mun, Jong-tak Lee, Jae Young Bae*

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Liquid repellency treatment has many applications in various sectors including self-cleaning surfaces. In recent research, it was confirmed that fluoride group on a surface had hydrophobic and oleophobic properties. Polysilsesquioxanes (PSSQs) were prepared by hydrolysis and condensation polymerization using various tri-functional alkoxide silane having a T^3 structure. In this study, Trifluoropropyltrimethoxysilane was used as a precursor, Fluorine functionalized PSSQs (F-PSSQs) of ladder structure were prepared by controlling silane concentration and pH at the solution. F-PSSQs were analyzed by ^{29}Si -NMR to observe the T^2 and T^3 peaks. The crystal lattice of products was confirmed by XRD analysis and a molecular weight of F-PSSQs was compared with the molecular weight of predicted structure by MALDI-TOF.

Poster Presentation : **MAT.P-513**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Crystal structure and ionic conductivity of new NASICON-type compounds

Minseong Kim, Jaegyeom Kim, Seung-Joo Kim*

Department of Energy System Research, Department of Chemistry, Ajou University, Korea

Framework oxides based on sodium (Na) super ionic conductor (NASICON) structure deserves further attention towards tailoring new lithium-ion conductors for application as electrolytes in solid state lithium batteries. In this study, $\text{Li}_{1+x}\text{Mg}_{(2+x)/3}\text{Ta}_{(4-x)/3}(\text{PO}_4)_3$ ($0 \leq x \leq 1$) was synthesized by solid state reaction and their crystal structures were characterized by synchrotron powder X-ray diffraction. All the compounds are based on NASICON structure and exhibit two different structures depending on the x value. $\text{Li}_{1.0}\text{Mg}_{0.66}\text{Ta}_{1.33}(\text{PO}_4)_3$ crystallizes to trigonal structure with space group $P-3c1$ when $x=0$, $\text{Li}_{2.0}\text{MgTa}(\text{PO}_4)_3$ crystallizes to monoclinic structure with space group Pn when $x=1$. Through the calculation of the Bond Valence Energy Landscape Map, the lithium ion passage was forward to appear at an activation energy of 1.07 eV for $\text{Li}_{1.0}\text{Mg}_{0.66}\text{Ta}_{1.33}(\text{PO}_4)_3$, while the $\text{Li}_{2.0}\text{MgTa}(\text{PO}_4)_3$ has an activation energy of 0.90 eV. The cyclic voltammetry results show that the reduction potential is 1.4eV, which is lower than that of other NASICON structure compounds such as $\text{LiTi}_2\text{Al}(\text{PO}_4)_3$. The ionic conductivity of $\text{Li}_{1.1}\text{Mg}_{0.7}\text{Ta}_{1.3}(\text{PO}_4)_3$ was confirmed to be the best ionic conductivity 1.18×10^{-3} S/cm.

Poster Presentation : **MAT.P-514**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Reversible Phase Decomposition-Formation of CaCrO_4

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Department of Energy System research, Department of Chemistry, Korea

The calcium chromate CaCrO_4 is decomposed to CaCr_2O_4 and CaO at high temperature (≤ 823 K) under a reducing atmosphere (with H_2 gas flow). The mixture of CaCr_2O_4 and CaO transforms aging to CaCrO_4 at high temperature (≤ 873 K) under oxidizing atmosphere (in the Air). Redox reaction of CaCrO_4 and CaCr_2O_4 proceeds reversibly. $\text{CaCrO}_4 \leftrightarrow \text{CaCr}_2\text{O}_4 + \text{CaO}$. The structure of $\delta\text{-CaCr}_2\text{O}_4$ has not been reported to data. Rietveld analysis based on high-resolution synchrotron X-ray powder diffraction data revealed that $\delta\text{-CaCr}_2\text{O}_4$ crystallized into a monoclinic symmetry (space group = $P 21/m$) with lattice parameters $a \approx 5.747 \text{ \AA}$, $b \approx 5.833 \text{ \AA}$, $c \approx 5.065 \text{ \AA}$, and $\beta = 105.79^\circ$. The synthesized CaCrO_4 was characterized by XRD, SEM, TGA-DSC and UV-vis spectroscopies.

Poster Presentation : **MAT.P-515**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Scattering Fourier Transform Biosensor (SFTB)

Sungwoo Lee, Sungjae Yoo, Hajir Hilal Khaleel Al Hammad, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

A binary mixture composed of Au nanospheres (Au NSs) and magnetically responsive nanoparticles (magnetic nanostirrer, MNS) for biosensing platform is reported. Through wet-chemical approach, highly uniform MNSs were synthesized by coating Au NSs with Pt layer and Ni layer, consecutively. Suspension of binary mixture of Au NSs and MNSs were modulated with external rotating magnetic field, which produced perturbed periodically fluctuating optical response due to the presence of Au NSs. As we control the concentration of Au NSs and surrounding refractive index, we can tune to intensity of plasmonic band, which leads to the change in perturbation on modulated light. Based on this, limit of detection was achieved as low as 5 pM of target analytes through bioassay, which were two orders of magnitude enhancement compared to LSPR spectral band shift assay.

Poster Presentation : **MAT.P-516**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fourier Transform Surface Plasmon Resonance of Magnetic Gyro-Nanodisks: Magnetic modulation and viscosity measurement at a localized area

Sang Baek Jung, Seongkeun Ih, Dajeong Kim, Jeongwon Kim, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

2-D noble metallic nanoparticles with localized surface plasmon resonance (LSPR) have attracted lots of attention in the field of therapeutics as well as sensors due to their unique properties and extensive applicability. Herein, we propose that the fabrication and application of magnetic modulatable and plasmonically active gyro-nanodisks(GNDs) for Fourier transform surface plasmon resonance (FTSPR) based viscosity sensing. These GNDs were precisely fabricated using the electrochemical deposition method with porous anodized alumina templates. Since these GNDs contain two plasmonically-active thin Au disks at each end, as well as the middle Ni segment responsive to an external magnetic field, periodic extinction signals can be generated under an external rotating magnetic field, which is converted from time domain to frequency domain using Fourier transformation. Moreover, an external magnetic field provided good remote control of the angular velocity and shear force, all of which is induced by the external rotating magnetic field which is controllable. Furthermore, Terminal frequency, defined as the available last signal frequency, is generated when the angular velocity is too high because of resistive forces between GND surface and fluid, the extinction of frequency signal decreased gradually because a certain portion of GNDs can't follow the rotating magnetic field. To understand and investigate their behavior enables us to study the viscosity of fluid (i.e the friction between GNDs and fluid.) As a proof of concept, a glycerol-water mixture was used as a variation of viscosity. These GNDs using FTSPR detected not only the viscosity of the bulk system of fluid but also localized fields at a micro-scale.

Poster Presentation : **MAT.P-517**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Blue Phosphorescence from Heptafluorosulfonyl Substituted Iridium Complexes

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The field of organic light emitting diodes (OLEDs) has been developed in the areas of solid-state lighting, large size and flexible displays. As emitting compound, phosphorescent materials can harvest both single and triplet excitons for light, enabling internal quantum efficiency of 100%. In particular, iridium complexes have been very successful as phosphorescent emitters, especially for green and red emissions, because of their high photoluminescent efficiency and short excited life time. However, development of high efficiency, especially deep-blue emitting phosphorescent materials has been a significant challenge for high performance of full color displays and white OLEDs. Therefore, there is a lot of work to find iridium complex that has both blue emission and high EQE in OLEDs. In this work, we designed and synthesized two heptafluorosulfonyl substituted Iridium complexes with perfluoro-sulfonyl group (SOCF7pic and SOCF7mpic) for blue phosphorescence organic light emitting diodes (PHOLEDs).

Poster Presentation : **MAT.P-518**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photoluminescence Enhancement of Ethanol with Graphene Quantum Dots Synthesized by Thermal Decomposition of Silicon Carbide

Naeun Lee

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Korea*

High-quality Graphene quantum dots (GQDs) with superior properties can be used advanced field. In particular, low cytotoxicity and large surface area of GQDs allowed to applicate GQDs in the bio-imaging fields. However, the complexity of their fabrication process and the overall quality of the GQDs need to be addressed when considering application. We report successful fabrication of high-quality GQDs by thermal decomposition of silicon carbide (SiC) under hydrogen etching gas. The fabricated GQDs were composed of high-quality graphene and H-terminated edges. PL emission spectrum with higher intensity was obtained in GQDs in ethanol solution since some of aromatic C=C in basal plane was destroyed and low defects were produced by invasion of oxygen functional group. The enhanced PL ratio was measured to be 27 and intrinsic emission was observed in GQDs. These results show possibility to apply at biosensing fields.

Poster Presentation : **MAT.P-519**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Research on Organic Semiconductors using a variable factor to self-assembly for Optoelectronic properties.

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In many research, self-assembly is useful tools for controlling of molecular distance. Most commonly used methods are π - π interaction and hydrogen bonding. In this study, we controlled two methods at the pin. We made a beta-sheet on the pin to break the conjugate, and the other method is an extension of the conjugate through a coupling. Structural differences of these molecules can affect different ways of stacking. In addition, the stacking can be controlled by changing the alkyl-chain of the side chains. Through this method, well deposited materials can be applied to organic electronic materials. To confirm this, it can be confirmed by NMR spectroscopy, Atomic Force Microscope(AFM), Scanning Electron Microscope(SEM), Transmission Electron Microscope(TEM), UV-visible spectroscopy and CV measurement.

Poster Presentation : **MAT.P-520**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

The anisotropy and metal to insulator transition behavior of VO₂ film deposited on C, R, M, A- crystal lattice plane of Al₂O₃.

Seong Cheol Hong, Myeongsoon Lee, Don Kim*

Department of Chemistry, Pukyong National University, Korea

The VO₂ films were prepared on C (0001), R (1-102), M(1-100), and A(11-20) plane of sapphire lattice. According the XRD analysis, all the films have highly anisotropic nature, the strong (011) reflection of random powder of VO₂ near $2\theta \sim 27^\circ$ is not appeared and shows strong (-211) and (021) reflections. Additionally, the VO₂ films deposited on the C, R, M and A plane have representatively anisotropic reflection of (020), (121), (-102) and (022), respectively. The morphology of the film also depends on the lattice plane of the surface, large particles on A, M, and R plane and small particles on C plane. The metal to insulator transition behavior of the films observed in IR transmittance and resistivity measurements do greatly affected by the used substrate, wide transition hysteresis on C plane ($\sim 30\text{K}$), but narrow and sudden transition on M, R and A plane ($\sim 8\text{K}$). We believe these change of the transition behavior is related with the lattice correlation between VO₂ and M, R and A plane of Al₂O₃ unstabilized the low temperature phase of the VO₂.

Poster Presentation : **MAT.P-521**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Carbohydrate detection of graphitized carbon nanotubes attached with gold particles fabricated by conversion of sucrose

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We have described simple and inexpensive carbohydrates detector, which is a field effect transistor (FET) consist of Au nanoparticles (AuNPs) attached graphitized carbon nanotubes (CNTs), which prepared through the carbonization of sucrose based on anodic aluminum oxide (AAO) template, without using any enzymes and catalysts. 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 will be compared with our previous AuNPs-MWCNT FET sensor, which have high sensitivity (3.4 mM^{-1} for sucrose and 6.9 mM^{-1} for glucose).

Poster Presentation : **MAT.P-522**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Detection of microcystin-LR by using a simple carbon nanotube@paper aptasensor

Myeongsoon Lee, Hak Jun Kim*, Don Kim*

Department of Chemistry, Pukyong National University, Korea

We have demonstrated a highly sensitive and selective aptasensor to detect microcystin-LR using assembly of DNA aptamer -multiwall carbon nanotubes (MWCNTs, diameter of 20 nm, length of 5 μm) and a micro-pore filter paper (pore size of 0.45 μm). Microcystin-LR (MCLR) is one of the most commonly detected and toxic cyclic heptapeptide cyanotoxins released by cyanobacterial blooms in surface waters, for which sensitive and specific detection methods are necessary to carry out its recognition and quantification. MWCNTs were activated with assembly of the microcystin aptamer (MCTA) by using N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC). The activated MWCNTs were deposited on the micro-pore filter paper to use as a aptasensor. The site selective interaction between MCLR and MCTA with an inexpensive bench top digital multimeter was monitored by resistance change.

Poster Presentation : **MAT.P-523**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Synthesis of Hollow Silver Cubes using Silver Oxide Mesoparticles as Templates and Their Morphological Evolution to Hexapods or Octapods

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Department of Chemistry, Chosun University, Korea

: In a previous paper, we introduced novel template-method for the synthesis of hollow silver hexapods using hexapod-shaped silver oxide mesoparticles. Experimental conditions for this synthesis is very subtle and the morphology of final product is susceptible to the concentration of reactant. Herein, we surveyed wide experimental condition to understand overall trend and morphological evolution of hollow silver hexapods. We will discuss evolutionary mechanism for the morphology of final product and suggest that silver cubes evolve to hexapods or octapods. Reference [1] J. Jo, S.-P. Cho, J. K. Lim*, Journal of Colloids and Interface Science 2015, 448, 208-214.

Poster Presentation : **MAT.P-524**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

One-pot synthesis of iron hydroxide hierarchical supraparticles

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¹*Chemistry, Chungnam National University, Korea*

Iron hydroxide nanomaterials are extensively explored in catalysis, sensors, environmental protection, energy storage and biomedical applications. In this work, two different hierarchical iron hydroxide supraparticles with mesoporous structures were obtained by a facile, efficient and environmentfriendly method via a sodium sulfate-assisted one-pot reaction. Particularly, no templates or toxic materials are involved. By controlling the ratio of iron ions and sodium sulfate, the structure of the iron hydroxide supraparticles can be smartly tailored from hierarchical porous one-dimensional hemp rope-like structure to three-dimensional iron hydroxide supraparticles. A plausible formation mechanism has been proposed based on systematic investigation of the assembly process.

Poster Presentation : **MAT.P-525**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Industrial-Scale Synthesis of Superparamagnetic Fe₃O₄ Nanoclusters for Bioseparation and Theragnostic Probes

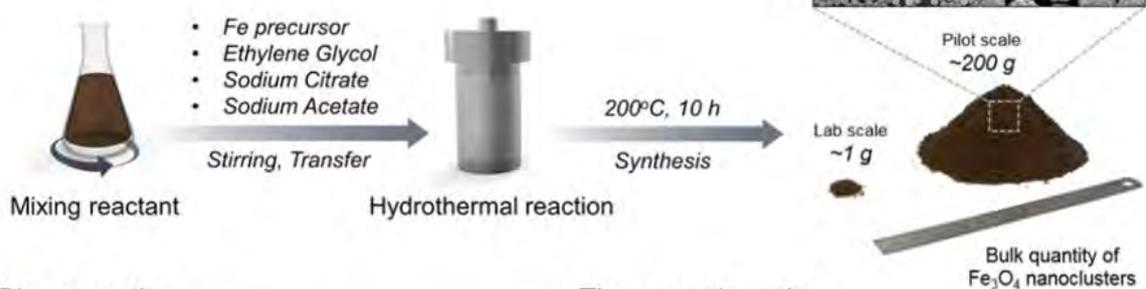
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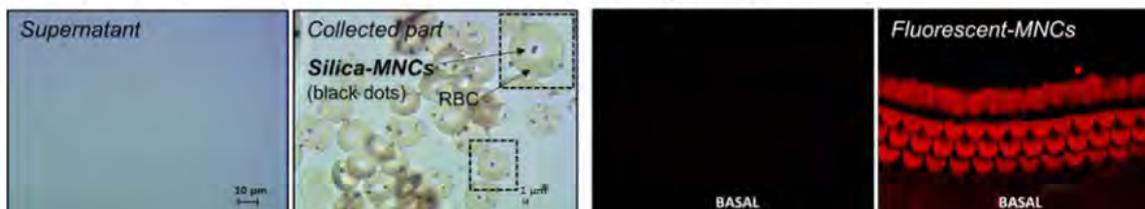
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Magnetic nanoparticles have had a significant impact on a wide range of advanced applications in the academic and industrial fields. In particular, in nanomedicine, the nanoparticles require specific properties, including hydrophilic behavior, uniform and tunable dimensions, and good magnetic properties, which are still challenging to achieve by industrial-scale synthesis. Here, we report a gram-scale synthesis of hydrophilic magnetic nanoclusters based on a one-pot solvothermal system. Using this approach, we achieved the nanoclusters with controlled size composed of magnetite nanocrystals in close-packed superstructures that exhibited hydrophilicity, superparamagnetism, high magnetization, and colloidal stability. The proposed solvothermal method is found to be highly suitable for synthesizing industrial quantities (gram-per-batch level) of magnetic spheres with unchanged structural and magnetic properties. Furthermore, coating the magnetic spheres with an additional silica layer provided further stability and specific functionalities favorable for biological applications. Using in vitro and in vivo studies, we successfully demonstrated both positive and negative separation and the use of the magnetic nanoclusters as a theragnostic nanoprobe. This scalable synthetic procedure is expected to be highly suitable for widespread use in biomedical, energy storage, photonics, and catalysis fields, among others.

Scalable synthesis of Fe_3O_4 Nanoclusters



Bio-separation



Poster Presentation : **MAT.P-526**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

A simple synthetic route for fct-FePd Nanocatalysts

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In this study, face-centered tetragonal (fct)-FePd magnetic nanocrystals (NCs) are developed to serve as artificial enzymes with high biocompatibility and reusability for the first time and are referred as “magnetozymes” (MagZs). The NCs were synthesized in an aqueous solvent via a one-pot method, using glutathione (GSH) and cysteine (Cys) as surfactants. The prepared hydrophilic fct-FePd MagZs are redispersible in water and their zeta potentials are in the range of 21.8–29.5 mV. The saturation magnetizations of the Cys- and GSH-MagZs are 4.7 and 41.4 emu g⁻¹, and both the MagZs exhibit superparamagnetism at 300 K. Further, they exhibit 2- and 7-fold enhancement in the catalytic activity for the inhibition of the production of reactive oxygen species induced by H₂O₂, respectively, than that of horseradish peroxidase. Computational simulation and electrochemical analysis indicate that the enhancement in the catalytic effect is due to the unique fct-structure of FePd MagZs as well as GSH and Cys protecting the MagZ surface. In vitro experiments reveal that the FePd MagZs clearly behave like a peroxidase and decrease reactive oxygen species levels in mammalian cells. The analysis of the cytotoxicity of FePd MagZs by exposing them to different cell lines over seven days indicates that they maintain >90% viability at concentrations up to 20 μg mL⁻¹. The FePd MagZs with high saturation magnetization and biocompatibility could potentially be applied as recyclable peroxidase-mimicking enzymes, antioxidizing agents, and biosensors in a variety of catalytic and biological applications.

Poster Presentation : **MAT.P-527**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Lining up Magnetic-Plasmonic Superparticles on Watery Substrate

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Large-area arrays of high aspect ratio and well-aligned linear magnetic nanochains are of remarkable research interest. However, the presence of various uncontrollable and competitive interactions to the magnetic ones creates complexity and uncertainty during the assembly process. A new approach for magnetic superparticle (SP) assembly over large areas (55×25 mm) is introduced using a combination of electrostatic and magnetic fields. Magnetic superparticles (Fe_3O_4 , $\text{Ag}@\text{Fe}_3\text{O}_4$ SPs) composed of hundreds of magnetite nanocrystals (10–20 nm diameter) are used as building blocks to fabricate arrays of high aspect ratio (up to 10^2) 1D linear nanochains. This assembly was induced by delicate co-assistance of magnetic and electrostatic forces so that the assembled structures can be firmly formed in large areas on any hydrophilic substrate within a few minutes. This assembly technique also minimizes the effects of thermal dynamics during evaporation, resulting in greater control over the assembled structures. The 1D magnetic array films exhibit strong optical polarization effects owing to their geometrical anisotropy, which can be used as a simple optical filter. Furthermore, by using $\text{Ag}@\text{Fe}_3\text{O}_4$ NPs as blocking unit, we fabricated a magnetoplasmonic nanochain array with tunable plasmonic properties by mechanical forces.

Poster Presentation : **MAT.P-528**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

In vivo feasibility test using transparent carbon nanotube-coated polydimethylsiloxane sheet at brain tissue and sciatic nerve

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¹*Chemistry, Chungnam National University, Korea*

Carbon nanotubes, with their unique and outstanding properties, such as strong mechanical strength and high electrical conductivity, have become very popular for the repair of tissues, particularly for those requiring electrical stimuli. Polydimethylsiloxane (PDMS)-based elastomers have been used in a wide range of biomedical applications because of their optical transparency, physiological inertness, blood compatibility, non-toxicity, and gas permeability. In present study, most of artificial nerve guidance conduits (ANGCs) are not transparent. It is hard to confirm the position of two stumps of damaged nerve during nerve surgery and the conduits must be cut open again to observe regenerative nerves after surgery. Thus, a novel preparation method was utilized to produce a transparent sheet using PDMS and multiwalled carbon nanotubes (MWNTs) via printing transfer method. Characterization of the PDMS/MWNT (PM) sheets revealed their unique physicochemical properties, such as superior mechanical strength, a certain degree of electrical conductivity, and high transparency. Characterization of the in vitro and in vivo usability was evaluated. PM sheets showed high biocompatibility and adhesive ability. In vivo feasibility tests of rat brain tissue and sciatic nerve revealed the high transparency of PM sheets, suggesting that it can be used in the further development of ANGCs.

Poster Presentation : **MAT.P-529**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Photo-induced Reversible Transformation of Azobenzene-containing MLD Films

Hyemi Lee, Jin seok Lee*

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Photo-responsive polymer film has been attracted in the field of material science including biological and optical application which are sensitive on the change of surface topology. Recently, azo compound (R-N=N-R'), as one of the photo-induced reversible transformation unit, has been highlighted and used in the polymer based biological and optical devices, because light used as external triggers is manageable to control without modification of nano-structures and environment concerns. In this study, we fabricated photo-reversible polyamide film based on coupling reactions between azobenzene-4, 4'-dicarbonyl dichloride (Azo) and hexamethylenediamine (HDA) by molecular layer deposition, and investigated the photo-switching behaviors of azobenzene-containing polyamide film. In situ Fourier Transform Infrared (FTIR) measurement was used to monitor the growth of polyamide film, and the orientation of chemical bondings in azobenzene-containing polyamide film was measured by plan-polarized grazing angle FTIR spectroscopy. In addition, we investigated the photo-induced reversible transformation of azobenzene-containing polyamide film using UV-vis spectroscopy.

Poster Presentation : **MAT.P-530**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Organometallic Compound Inserted Layered Clays for Enhanced Water Oxidation

Jae Ryeol Jeong, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

As an environmentally friendly energy resources, hydrogen fuel production via photoelectrochemical or electrochemical water splitting have gotten huge attraction for decades. Tremendous efforts have been devoted to realize spontaneous hydrogen energy production, however, slow kinetics of oxygen evolution reaction (OER) are major huddles need to overcome. In order to figure out the retardation of OER, heterogenous and homogeneous electrocatalysts with decreased overpotential have been developed. However, 250 mV overpotential have been considered as a limitation for decades. In this researches, organometallic complexes inserted layered clay minerals studied as an OER catalysts to utilize advantage of heterogenous and homogeneous catalysts. Various transition metal based-organic complexes could be easily switched, and we could screen best hybrid catalysts. Thanks to synergistic effects of high reactivity of organometallic complexes for OER and stabilization of organometallic compounds in the clay minerals, the overpotential for OER could be reduced by 180 mV at the current density 5 mA/cm² in the Co-complexes inserted clay minerals. Also, the catalysts maintain its OER catalytic performance over 10 hours. This research was supported by Creative Materials Discovery Program (NRF-2017M3D1A1039379) through the National Research Foundation of Korea(NRF) funded by Ministry of Science and ICT.

Poster Presentation : **MAT.P-531**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Fabrication of Water-repellent Polymeric Film by Spray Coating of Hydrophobic Nanoparticles

Young-Sang Cho*, **Sol Jeong**, **Soyoung Nam**

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

In this presentation, low-cost fabrication method on PDMS-based polymeric film with water-repellent surfaces will be discussed. Colloidal dispersion of hydrophobic silica nanoparticles was prepared wet chemical modification of the nanopowder using silane or titania coupling agent. The chemisorbed coupling agents on the nanoparticle surface was confirmed by FT-IR analysis. After sonication, the resulting hydrophobic particles were suspended in alcohol medium. To prepare water-repellent film, lotus effect was induced by transferring micron-sized surface protrusions of commercial paper on PDMS film. Surface roughness of the resulting rough PDMS surface was measured by surface profile tester. The resulting rough PDMS surfaces were spray coated with hydrophobic silica nanoparticle dispersion to increase the contact angle of water droplets by lotus effect. The maximum contact angle of water droplets was higher than 145 ° with nearly superhydrophobic property. The effect of the number of spray coating and type of coupling agent were also studied by measuring the static contact angle of water droplets. Acknowledgments: This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2017R1C1B5017174) and the Industrial core technology development program (10077545, Development of icephobic coating materials for extreme environment) funded by the Ministry of Trade, Industry & Energy (MI, Korea).

Poster Presentation : **MAT.P-532**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Excitation intensity dependent photoluminescence property of perovskite type quantum dots

Sang Woong Kang, Jeong Yoon Choi, Chan Im*

Department of Chemistry, Konkuk University, Korea

Cesium lead halide perovskite (CsPbX_3 , $X = \text{Cl, Br, I}$) quantum dots (QDs) and their partly Mn substituted QDs ($\text{CsPb}_{1-x}\text{Mn}_x\text{X}_3$) gather attention due to their unique photoluminescence (PL) efficiencies. To understand their solid-state-induced exciton dynamics of the QDs, two types of QDs having different PL decay dynamics were investigated as in a form of aggregates. Furthermore, those behaviors were characterized upon degradation to achieve practical applications by using those promising QDs. To obtain their deeper insights related with long-term stability of their aggregated solid-states we comparatively studied the CsPbX_3 and the $\text{CsPb}_{1-x}\text{Mn}_x\text{X}_3$ type QDs being stocked longer than 50 days under dark ambient condition by means of excitation intensity dependent time-resolved PL spectroscopies. Those investigations are performed with their powder samples in addition to their diluted and concentrated solutions to depict the influence of the inter-QD interaction of the aged QD aggregates on their radiative decays by using various excitation intensities which are important for their solid-state applications. This work was supported by the National Research Foundation of Korea (Project No.: NRF-2018K2A9A2A06023902).

Poster Presentation : **MAT.P-533**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Incorporation of TiO₂ Nanoparticles onto Carbon Nanotube Fibers: UV Resistant Property and Photocatalytic Applications of TiO₂/Carbon Nanotube Nanocomposite Fibers

Chul jun Yoon, Youngkwan Kim^{1,*}, Kyoungsoo Kim²

Chonbuk National University, Korea

¹*Korea Institute of Science and Technology, Korea*

²*Department of chemistry, Chonbuk National University, Korea*

Carbon nanotube (CNT) fiber has interesting physicochemical properties such as low density, chemical inertness, excellent mechanical properties and high electrical conductivity. Because of those properties, CNT fiber is regarded as a promising material for developing next-generation high-performance fibers beyond carbon fibers which are widely used for aerospace, defense and automobile industries. For realistic application of CNT fibers, it is highly demanded to improve their long-term stability under harsh conditions because the operating conditions of CNT fibers are generally extremely harsh such as strong radiation and high temperature. Titanium oxide (TiO₂), well known a wide-bandgap semiconductor, exhibits interesting properties to improve the stability of CNT fibers based on its high UV absorbance and thermal stability. In this study, we develop an efficient strategy to coat CNT fibers with TiO₂ for improvement of their long-term stability under UV irradiation. TiO₂@CNT fibers showed highly-sustainable mechanical and electrical properties compared to pristine CNT fibers under exposure to a strong UV light at high temperature. In addition, TiO₂@CNT fibers showed a high photocatalytic activity enough to degrade organic pollutants.

Poster Presentation : **MAT.P-534**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Optical fibers/Red TiO₂ nanotubes for Trace Contaminant Control System

Hyun Kim, Bee Lyong Yang*

School of Advanced Materials Science and Engineering, Kumoh National Institute of Technology, Korea

The concentration of volatile organic compounds (VOCs) that are off-gases from instruments as well as from the human metabolism are significantly considered when designing of spacecraft and spacesuit for long period mission such as planet exploration because they derive diseases such as central nervous disorder, irritation of mucosa and arrhythmia. As present VOCs control system that are composed 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 and complex, thus, development of compact and efficient VOCs control system is important. As a results, we suggested that TiO₂ nanotubes enable to reduce weight of present VOCs control system and hazardous LiOH replacement. In this study, TiO₂ nanotubes were used for decomposition of VOCs that confined at inside and outside tube walls to protect astronauts against VOCs. TiO₂ nanotubes were prepared by alkaline based hydrothermal reaction in convection oven and subsequently it was processed on TiO₂ nanotube ink. 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 and transparent glass sheets will be investigated and evaluated in the trace contaminant system of spacecrafts.

Acknowledgement

This research was supported by space Core Technology Development Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education Science and Technology(MEST) (2017M1A3A3A02016666)

Poster Presentation : **MAT.P-535**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

g-C₃N₄/CuNi/CaFe₂ photo-cathode for CO₂ photo-conversion

Hyun Kim, Bee Lyong Yang*

School of Advanced Materials Science and Engineering, Kumoh National Institute of Technology, Korea

Research of CO₂ fuel conversion selectivity have been critical issue because products are mixed during CO₂ photo-conversion. Some of metal oxide catalysts to improve conversion selectivity have been available for different products. In this study, CaFe₂O₄ photo-cathode was prepared by polyol method, chemical bath deposition and oxidation after electrodeposition using FTO glass. Grown heterojunction nano-structures were confirmed by means of both FESEM (field emission scanning electron microscope) and TEM (transmission electron microscope). CO₂ to CH₃OH conversion selectivity 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 NMR (nuclear magnetic resonance) and Raman spectroscopy to identify inside solution composition. Quantitative measurement of CH₃OH was evaluated by GC-MS (gas chromatography-mass spectrometer) and stability of CaFe₂O₄ also was studied.

Acknowledgement

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education Science and Technology(MEST) (2018R1D1A1B07040352)

Poster Presentation : **MAT.P-536**

Material Chemistry

Exhibition Hall 2, FRI 11:00~12:30

Pulsed wire evaporation based CuNiAl for CO₂ to CH₃OH selectivity and high yield

Hyun Kim, Bee Lyong Yang*

School of Advanced Materials Science and Engineering, Kumoh National Institute of Technology, Korea

Ongoing research of the precise CO₂ to fuel conversion selectivity became important issue because products are mixed during CO₂ reduction. In order to improve conversion selectivity, some of metal oxide catalysts are available for different products. In this study, InP was vertically grown on FTO glass by chemical bath deposition instead of dominant chemical vapour deposition. And grown InP nanorods were confirmed by means of both FESEM (field emission scanning electron microscope) and TEM (transmission electron microscope). Cu₂O NPs were comparatively studied by two different methods that of electrodeposition/oxidation process and SILAR (successive ionic layer adsorption and deposition process). CO₂ to CH₃OH conversion selectivity 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 NMR (nuclear magnetic resonance) and raman spectroscopy to identify inside solution composition. Quantitative measurement of CH₃OH was also conducted by HPLC (high performance liquid chromatography).

Poster Presentation : **ELEC.P-436**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Novel Propionitrile based electrolyte system for electrochemical double layer capacitors to enhance cycle stability at 3.5V

Thi Hoai Van Nguyen, Kyung-koo Lee^{1,*}

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To increase the cyclic ability of a portable device such as electrochemical double layer capacitors (EDLCs), different electrolyte systems have been tested. Here, Propionitrile (PN) electrolyte has been investigated with different quaternary ammonium salts (TEABF₄, SBPBF₄, and SP2BF₄) and compared with well-known commercial electrolyte acetonitrile (ACN). ACN has high power density and cycle life at an operative voltage 2.7-2.8 V but PN showed better performance and cyclic ability at a higher voltage (3.5 V). The electrochemical performances i.e. galvanostatic charge-discharge (GCD), cyclic voltammetry (CV) and physical properties i.e. ionic conductivity, viscosity of these two electrolytes was carried out in activated carbon electrode based coil cells. Although the decreased conductivity and increased viscosity were observed, PN significantly enhances the cyclic ability of EDLCs and exhibit excellent performance at high voltage (3.5V).

Poster Presentation : **ELEC.P-437**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Time transient electrochemical monitoring of tetraalkylammonium polybromide solid particle formation: observation of ionic liquid-to-solid transitions

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Department of Chemistry, Hanyang University, Korea

Energy storage systems (ESSs) using a Br^-/Br_2 redox reaction such as a Zn/Br redox flow battery (RFB) or a redox-enhanced electrochemical capacitor (Redox-EC) suffer from self-discharge reactions resulting in significant coulombic loss. To inhibit the self-discharge, quaternary ammonium (Q^+) and tetraalkylammonium (T^+) bromide are added to form ionic liquid (QBr_{2n+1}) and solid (TBr_3) polybromides during the ESS charging process. The electrochemical formation of liquid QBr_{2n+1} and its electrochemical properties have been examined. The detailed mechanisms of ionic solid TBr_3 formation, however, have not yet been explored. In this article, we analyzed the ionic liquid-to-solid phase transition of TBr_3 particles using a time transient electrochemical method. We suggest the formation of ionic solid TBr_3 particles via hydrated TBr_3 droplets as an intermediate phase, which are generated by electro-oxidation of Br^- in an aqueous TBr solution. We found the phase transition time of TBr_3 particles is strongly dependent on the chemical structure of T^+ and the concentration of TBr in an aqueous solution.

Poster Presentation : **ELEC.P-438**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Electrochemistry of dual-redox ionic solid complexes: understanding their formation and redox-chemistry via proton coupled electron transfer (PCET)

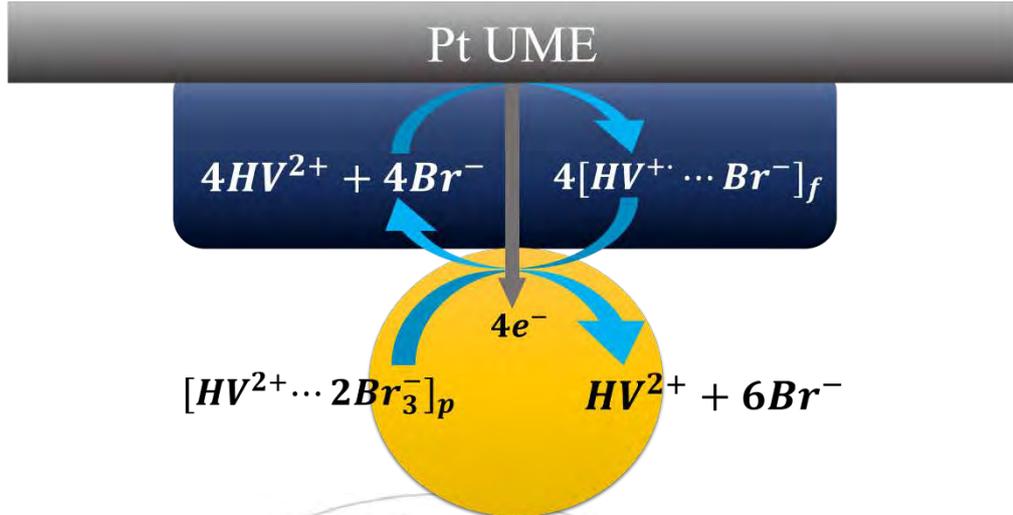
Semi Lee, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Here we present the electrochemistry based on the formation/dissolution reactions of two dual-RICs(Redox ionic complexes) : HV^{2+} and Br^- . During a charge process, HV^{2+} is reduced to form a solid $[HV^+ \cdot Br^-]$ on an anode, while Br^- is oxidized to form a solid $[HV^{2+} \cdot 2Br_3^-]$ on a cathode, resulting in significant suppression of self-discharge in the Redox-EC(electrochemical capacitors). We found that $[HV^+ \cdot Br^-]_{(s)}$ formed on Pt UME is electrochemically further reduced through proton coupled electron transfers (PCETs). Also, we deciphered stochastic current spikes associated with the galvanic exchange reaction between a $[HV^+ \cdot Br^-]_{(s)}$ film and a $[HV^{2+} \cdot 2Br_3^-]$ particle in an acidic and neutral solution, and proposed the different electro-reduction mechanism of $[HV^{2+} \cdot 2Br_3^-]$ particles on a modified Pt UME with $[HV^+ \cdot Br^-]$ in acidic condition from that in a solution with neutral pH.

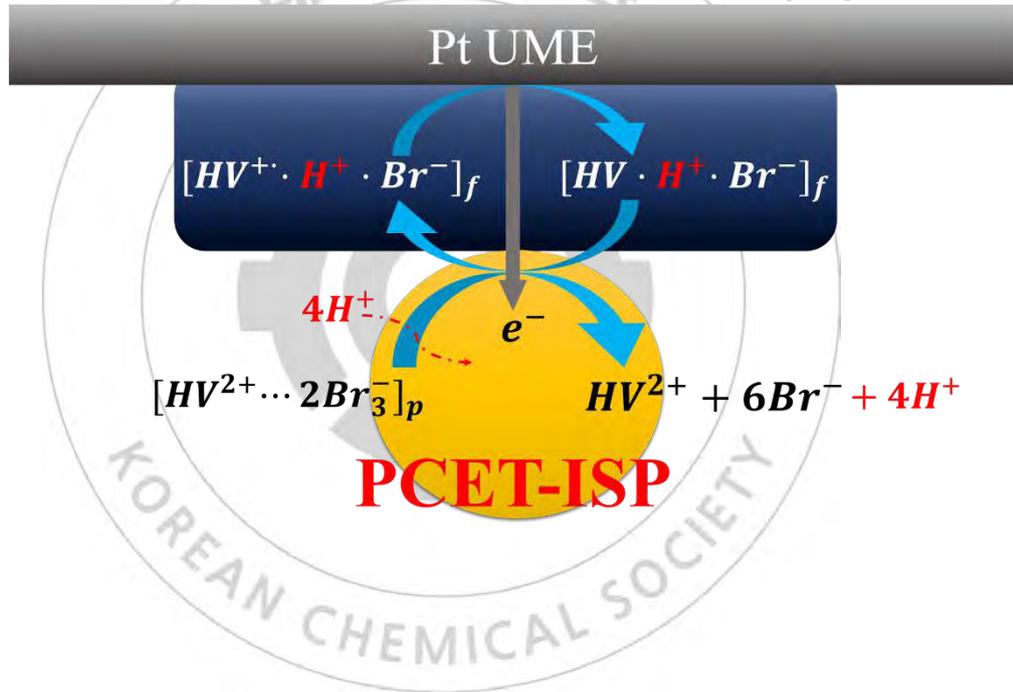
(a) In 0.33 M Sodium Sulfate Solution

When the negative potential is biased



(b) In 1 M Sulfuric Acid Solution

When the negative potential is biased



Poster Presentation : **ELEC.P-439**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Activating MoS₂ basal plane with Ni₂P nanoparticles for Pt-like hydrogen evolution reaction

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Electrocatalytic water splitting has great importance for sustainable hydrogen production due to its high purity and environmental-friendly process. The development of an efficient and non-noble metal cheaper catalyst for sustainable hydrogen generation is highly desirable to meet future energy challenges. Due to its inert basal plane, the molybdenum sulfide displays relatively poor performance in acidic media. Here we activate the MoS₂ basal planes by growing Ni₂P nanoparticles on it. The Ni₂P/MoS₂ heterostructure is constructed via in-situ phosphidation of an indigenously synthesized NiMoS₄ salt as a single precursor to form a widely cross-doped and chemically connected heterostructure. As a result, the Ni₂P/MoS₂ heterostructure grown on N:RGO or N:CNT displays Pt-like HER performance in acidic media, outperforming the incumbent best HER electrocatalyst, Pt/C, in a more meaningful high current density region (>200 mA/cm²) making them a promising candidate for practical water electrolysis applications.

Poster Presentation : **ELEC.P-440**

Electrochemistry

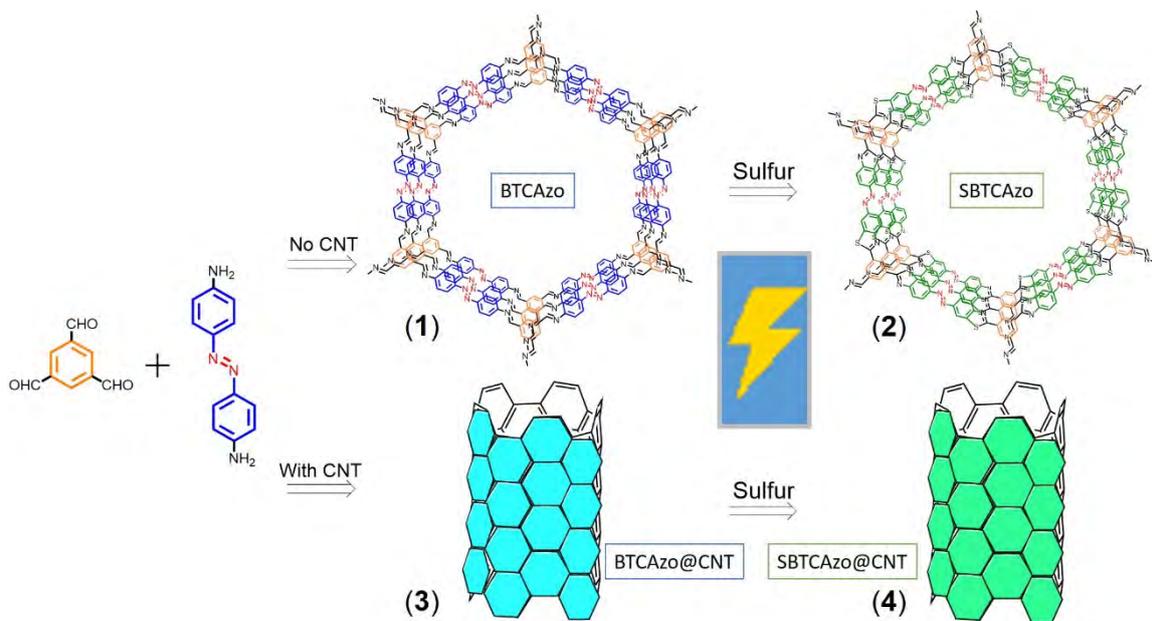
Exhibition Hall 2, THU 11:00~12:30

Evaluation of Azo-based, Redox-Active Covalent Organic Frameworks as positive electrode materials in Organic Lithium Ion Battery

Vikram Singh, Bora Kang, Hye Ryung Byon*

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

The key to organic-based lithium-ion batteries (OLIBs) is efficient trigger of redox-active moieties and reduced solubility of organic molecules in aprotic electrolytes. Covalent organic frameworks (COFs) offer porosity, high crystallinity, chemical stability and insolubility. Coupled with an ability to selectively position redox-active building blocks render COFs as strong alternatives to small molecules. In this work, redox-active Azo groups (-N=N-) are incorporated into novel imine-linked COFs (1) and tested as positive electrode materials in OLIBs. 1 is post-synthetically modified to thiazole-linked COFs (2) to strengthen the framework under (electro-)chemical stress and to synergistically improve electrical conductivity. Few layer COFs are grown over multiwalled carbon nanotubes (3 and 4) for improved redox-activity and conductivity. 3 and 4 have similar backbone as in 1 and 2, respectively. All COFs required initial activation performed by means of cyclic voltammetry. 1 and 3 with imine-linkage showed unsatisfactory cyclability and rate capability in 1-3 V range, either at low (10 mA g^{-1}) or high (200 mA g^{-1}) current densities. 2 and 4 displayed clear redox behavior attributed to lithiation/delithiation of azo groups with a stable capacity of ~200 mA $h g^{-1}$ at 10 mA g^{-1} . Further, remarkable cycling stability (> 100 cycles) at 100 mA g^{-1} and excellent rate capability (10 to 200 mA g^{-1}) was achieved with 2 and 4. The thiazole moiety in the COF skeleton improves the chemical stability and we hypothesize a synergistic role of S-atom in the activation of azo groups towards redox activity with respect to Li/Li $^{+}$. Ex-situ and operando-Raman spectroscopic analysis confirmed the involvement of azo groups in reversible lithiation/delithiation process in 2 and 4 based OLIBs.



Poster Presentation : **ELEC.P-441**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

FeF₂ Nanoparticles Wrapped in Graphitic Carbon Prepared from Fe-MIL-88B Template as a Cathode Material for Sodium-Ion Batteries

Achmad Yanuar Maulana, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

In recent years, the advancement of lithium-ion batteries (LIBs) has grown and become the leading power supplying devices for electric vehicles and portable electronic devices. However, the limited resources and geographical distribution issues of lithium will make LIBs inappropriate to be utilized in large-scale applications such as energy storage systems (ESS) and smart energy grids. As an effort of exploring the breakthroughs, sodium-ion batteries (SIBs) have been attracted because of the high abundance, low-cost, and similar redox reactions of sodium compared to lithium. However, the exploration of high-performance electrode materials is still necessary. Iron difluoride (FeF₂) has been considered as one of the most suitable cathode materials for SIBs due to its economic merit, abundance, and high theoretical capacity (about 571 mAh g⁻¹). Unfortunately, FeF₂ has often suffered low reversible capacity and cycling stability because of its poor electrical conductivity. In this work, FeF₂ nanoparticles wrapped in graphitic carbon (FeF₂@GC) was successfully synthesized from Fe-containing metal-organic framework, Fe-MIL-88B. FeF₂@GC discharged high initial capacity of about 611.4 mAh g⁻¹ with superior cycling stability in long cycles at a current density of 50 mA g⁻¹.

Poster Presentation : **ELEC.P-442**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Layer-by-layer growth of CIGS/CdS architecture on Mo substrates by E-ALD

Mukunthan Ramasamy, ChanYong Jung, Yu-Beom Yeon, Chi-Woo Lee*

Department of Advanced Materials Chemistry, Korea University, Korea

CuIn_xGa_(1-x)Se₂ (CIGS) is a chalcopyrite p-type semiconductor compound which are largely known for its explicit properties of highly adjustable bandgap (1.04 eV for CuInSe₂ (x = 0) to 1.68 eV for CuGaSe₂ (x = 1)), bandgap found at optimum conversion efficiency range (1.4 ~ 1.5 eV), high absorption coefficient (1×10⁵ cm⁻¹), and the material is highly stable under high energy irradiation. Cadmium sulfide (CdS), an n-type semiconductor compound with the band gap of 2.4 eV, good optical transmittance and low resistivity makes this compound a noble candidate as a buffer layer in thin-film photovoltaic cells. This CIGS-CdS duo offers the highly efficient CIGS thin-film solar cells available in the market today. The electrochemical atomic layer deposition (E-ALD) which is an electrochemical version of the ALD method, is adopted for making the homogeneous layers of Cu-In-Ga-Se and Cd-S semiconductor compounds on Mo substrate. The E-ALD works under the principle of surface limited reactions (SLRs) which is referred to as underpotential deposition (UPD) in the electrochemical process. The UPD process takes place under or less than the Nernst potential; where an atomic layer formed as the result of the free energy formation of a surface compound. The specific UPD potentials were determined by cyclic voltammetry (CV) studies in respect with each electrolyte solutions. Series of alternate cycles of deposits were performed to form the preferred film with precise stoichiometry. The synthesized films were analyzed by X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and the PEC experiments. The photoelectrochemical (PEC) studies of a photovoltaic (PV) film could reveal the semiconductive nature of the absorber layer and absorber/buffer film architecture in fast basis. The photoelectrochemical behavior of each layer of the device is important to make the PV cell a defect-free during the device making process. This important technique could help the researcher to analyze the stability of the materials against light irradiation and could lead to improving the materials property.

Poster Presentation : **ELEC.P-443**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Spontaneously adsorbed platinum complex on Au-quartz via EQCM

ChanYong Jung, Chi-Woo Lee*

Department of Advanced Materials Chemistry, Korea University, Korea

We have conducted studies to improve the usability of Pt, which is highly valuable as a catalyst. The addition of platinum complex solution to the aqueous solution where Au-quartz was located results in spontaneous and irreversible adsorption of the PtCl_4^{2-} complexes. Pt has been used as catalysts in many important chemical reactions for long time and is the most important single catalyst for oxygen reduction and hydrogen oxidation in fuel cells. Electrochemical deposits produced from the reduction of platinum complexes in aqueous solutions of platinum complexes on the model surface of gold electrode has been investigated to study the mechanistic aspect of the reactions. Contrasting behaviors were reported in the literature but the quantitative aspect of adsorption is lacking.



Poster Presentation : **ELEC.P-444**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

A comparative study of ZnS film fabricated by CBD and ALD

Yu-Beom Yeon, Jungho Choe¹, Chi-Woo Lee*

Department of Advanced Materials Chemistry, Korea University, Korea

¹*Control and Instrumentation Engineering, Korea University Sejong Campus, Korea*

Solar energy is a renewable energy source. This means that we cannot run out of solar energy, as opposed to non-renewable energy sources (e.g. fossil fuels, coal and nuclear). The potential of solar energy is beyond imagination. The surface of the earth receives 120,000 terawatts of solar radiation (sunlight) – 20,000 times more power than what is needed to supply the entire world. CdS and ZnS have large band gap energy. (CdS : 2.4eV, ZnS : 3.7eV) Because of this feature, it can serve as a buffer layer in the cell and is useful in solar cells. The electrodeposition method is a method of forming a thin film by dissolving a component material in a supporting electrolyte solution and then using an electrochemical oxidation / reduction reaction. The advantage of the electrochemical method is that it has less waste of raw materials, minimizes the generation of wastewater, and is more easily tailored to the reaction conditions than other methods. The CBD (Chemical Bath Deposition) method is advantageous in that the manufacturing process is relatively simple as compared with other methods, the manufacturing cost is low, and the reproducibility is excellent. In this study, ZnS was electrodeposited on FTO Glass by ALD (Atomic Layer Deposition) and CBD (Chemical Bath Deposition) method. Electrochemical electrodeposition was performed using PGSTAT302N from Echem-Technology, and the layer was increased using AECS (Automatic Chemical Experiment System). ZnS thin films were analyzed by XRD (X-ray Diffraction), SEM (Scanning Electron Microscope) and EDS (Energy Dispersive Spectroscopy).

Poster Presentation : **ELEC.P-445**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Revisit V(V)-V(IV)-V(III)-V(II) electrochemistry in highly concentrated acidic medium: origin of parasitic hydrogen evolution reaction (HER)

Jihye Lee, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

We present the through voltammetric analyses associated with V(V)-V(IV)-V(III)-V(II) redox chemistry occurring in highly concentrated mixed acidic medium based on digital voltammetric simulation for understanding electrochemistry in high energy density VRFB. Virtually, the proposed mechanism of $\text{VO}_2^+/\text{VO}_2^{2+}$ and $\text{V}^{3+}/\text{V}^{2+}$ redox reactions on a carbon electrode are well described in each elementary steps. However, the proposed mechanistic pathway was remained questionable because, as the authors' best knowledge, we could not find the reports to prove or identify the proposed reaction pathway through voltammetric analyses based on the thorough investigation from the digital voltammetric simulation. In addition, it has been known that hydrogen evolution reaction (HER) occurs as the side reaction during electro-reduction of V^{3+} in VRFB, which decline the coulombic efficiency of VRFB due to the partial consumption of charge during the charge process. In spite of the importance of understanding the origin of the parasitic HER occurring in VRFB, only a few articles have been reported, and therefore, main reason for this critical side reaction is still unrevealed. we found the generation of V(II) species as the side reaction, which could act as an electrocatalyst for HER, and this V(II) species could only exist when V^{3+} is electrochemically reduced on a glassy carbon electrode resulting in high local concentration of V^{2+} in the vicinity of the electrode surface. This vanadium catalyst disappears when the local high concentration of V^{2+} disappears and the catalyst effect disappears. This reaction is called the 'phantom effect'. This 'phantom' effect of V(II) species could be also well explained based on the suggested mechanism. This effect occurs when the starting material of the reaction is $\text{V}(\text{IV})\text{O}_2^+$ or $\text{V}^{3+}(\text{III})$. These starting materials can be reduced by electrochemical methods such as chronoamperometry or cyclic voltammetry to confirm the HER catalyst effect and phantom effect.

Poster Presentation : **ELEC.P-446**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Cobalt Oxide Nanocrystals for Electrochemical and Photoelectrochemical Water Splitting

Hye Rin Choe, Ki min Nam*

Department of Chemistry, Pusan National University, Korea

Spontaneous phase transition of wurtzite-CoO to spinel-Co₃O₄ was progressed on various substrates in the presence of water, resulting in efficient chemical bonding between the Co₃O₄ and the substrate without binder material. The proficient interaction of Co₃O₄ with the conductive substrate was suitable for the electrochemical water oxidation reaction. Furthermore, the Co₃O₄ was deposited on a semiconductor (BiVO₄ photoelectrode) via the phase transition of wurtzite-CoO to investigate the proficient integration of the electrocatalyst onto a photoelectrode. The BiVO₄/Co₃O₄ composite improved photoelectrochemical water oxidation activity, due to the efficient and subsequent interaction between the BiVO₄ and Co₃O₄. Based on the electrochemical and photoelectrochemical water oxidation results, the reported spontaneous phase transition of wurtzite-CoO to Co₃O₄ has great potential applications for electrochemical catalytic reactions.

Poster Presentation : **ELEC.P-447**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Bi₂O₃/Bi₂S₃ Composite for Efficient Photoelectrochemical Reaction

Jihyeon Kim, Ki min Nam*

Department of Chemistry, Pusan National University, Korea

The Bi₂O₃/Bi₂S₃ composite was synthesized via an in-situ sonochemical reaction. The in-situ growth of Bi₂S₃ provides a good interaction with the Bi₂O₃ layer. The resulting Bi₂O₃/Bi₂S₃ composite showed enhanced photoelectrochemical (PEC) activity compared to those of the other Bi₂S₃ electrodes. These enhanced levels of activity mainly originate from two factors: (1) the enhanced charge separation of Bi₂S₃ on the Bi₂O₃ layer due to the CB and VB of Bi₂O₃ being more positive than those of Bi₂S₃, which are favorable for the charge separation of Bi₂S₃, and (2) the effective composite interface with less interfacial defects by the in-situ growth method. These findings provide important guidance for the design of highly efficient electrodes, particularly bearing on hetero-structures, for enhanced PEC performances.



Poster Presentation : **ELEC.P-448**

Electrochemistry

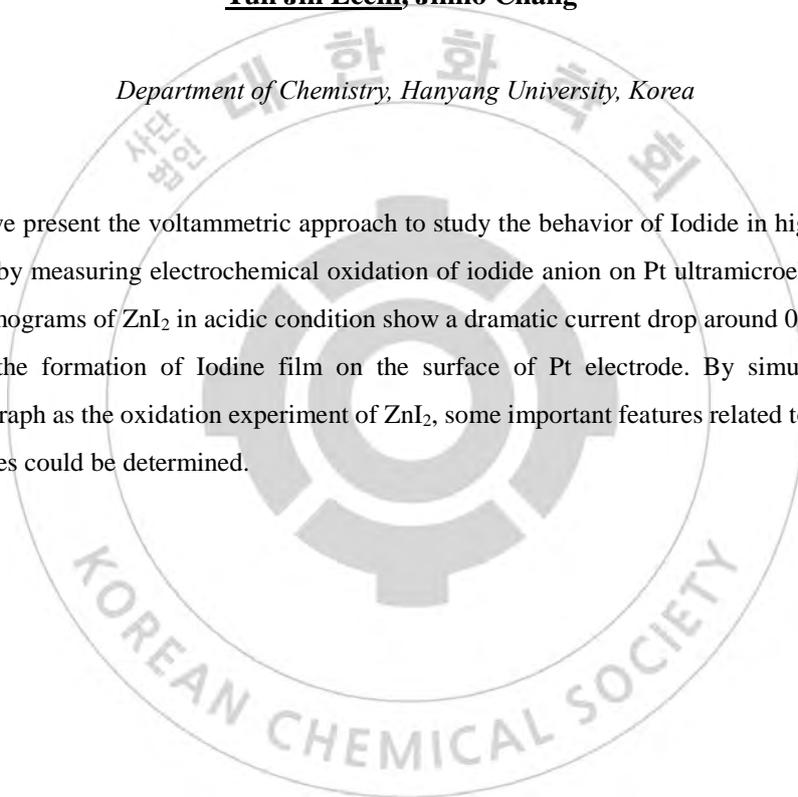
Exhibition Hall 2, THU 11:00~12:30

Study of the anodic behavior of Iodide in high concentration ZnI_2 media by steady state voltammetry on Pt ultramicroelectrode

Yun Jin Leem, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

In this study, we present the voltammetric approach to study the behavior of Iodide in high concentration ZnI_2 solutions by measuring electrochemical oxidation of iodide anion on Pt ultramicroelectrode (UME). Cyclic voltammograms of ZnI_2 in acidic condition show a dramatic current drop around 0.4V which could be related to the formation of Iodine film on the surface of Pt electrode. By simulating the same voltammetric graph as the oxidation experiment of ZnI_2 , some important features related to such behaviors of Iodide species could be determined.



Poster Presentation : **ELEC.P-449**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Polymer Chain Growth Analysis Using Electrochemical Method on an Ultramicroelectrode: Relationship between Viscosity and Molecular Weight

Hae-Young Kim, Byung-Kwon Kim*

Department of Chemistry, Sookmyung Women's University, Korea

Herein, for the first time, the cyclic voltammetry study for the viscosity of polymer solution has been reported. To follow the conversion of the polymer increase, high viscosity of solution hindered diffusion of redox species, resulting in the steady-state current decrease. All of the electrochemical experiments were conducted on an Au ultramicroelectrode (UME). Polymer was synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization using methyl methacrylate (MMA), and the polymerization results confirmed with NMR spectroscopy and gel permeation chromatography. The relationship between molecular weight of polymer and viscosity of solution was also investigated.

Poster Presentation : **ELEC.P-450**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Electrochemical behavior analysis of microbeads in aqueous and organic solution

Yeji Kang, Byung-Kwon Kim*

Department of Chemistry, Sookmyung Women's University, Korea

The microbeads, uniform polymer particles, are usually used in personal care and biotechnology. They are easily modified by various functional group, which makes the beads have different properties, such as protein affinity and fluorescent expression. It can be useful in biotechnology, but hazardous in environmental systems. Therefore, fast and easy detection of microbeads in various condition is important. The electrochemical method is proper to detect and find out properties of microbeads. Therefore, the electrochemical behavior in two type of solutions with same redox molecules are studied. These are performed by chronoamperometry measurement with ultramicroelectrode(UME). The experimental results show different signals according to the type of solution. In this study, we tried to find out the reason of these different behavior in two type of solutions.

Poster Presentation : **ELEC.P-451**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

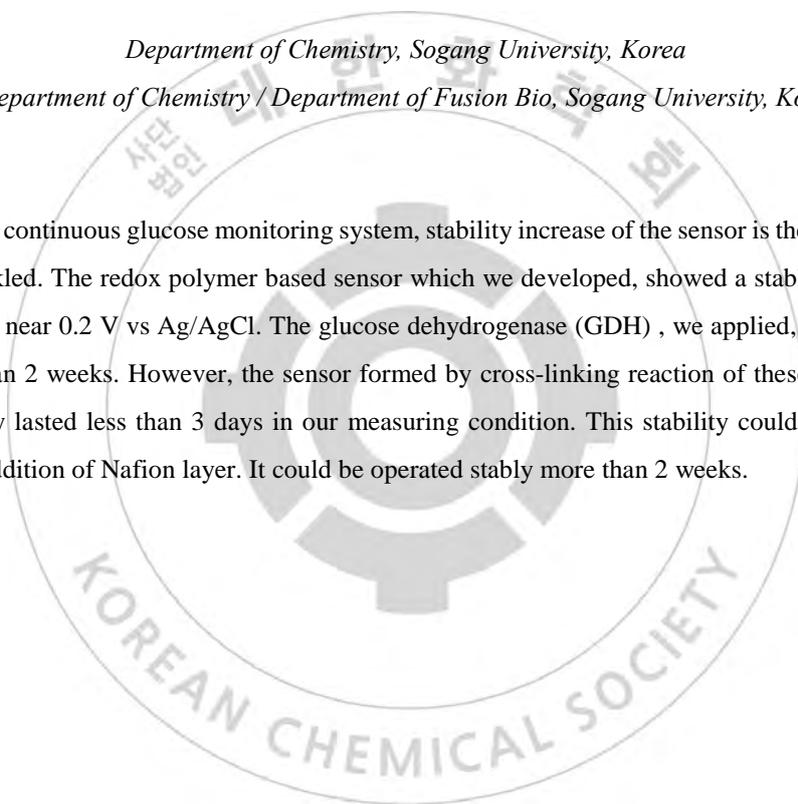
Stability Increase of Glucose Sensor by addition of nafion layer

Eunhyeon Ha, Woonsup Shin^{1,*}

Department of Chemistry, Sogang University, Korea

¹*Department of Chemistry / Department of Fusion Bio, Sogang University, Korea*

For developing continuous glucose monitoring system, stability increase of the sensor is the most important point to be tackled. The redox polymer based sensor which we developed, showed a stable and reversible redox behavior near 0.2 V vs Ag/AgCl. The glucose dehydrogenase (GDH), we applied, was found to be stable more than 2 weeks. However, the sensor formed by cross-linking reaction of these redox polymer and GDH, only lasted less than 3 days in our measuring condition. This stability could be dramatically increased by addition of Nafion layer. It could be operated stably more than 2 weeks.



Poster Presentation : **ELEC.P-452**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Affordable Fabrication of Conductive Electrodes and Dielectric Films for a Paper-based Digital Microfluidic Chip

Veasna Soum, Sooyong Park, Oh-Sun Kwon*, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

In order to fabricate a digital microfluidic (DMF) chip, which requires a patterned array of electrodes coated with a dielectric film, we explored two simple methods: Ballpoint pen printing to generate the electrodes, and wrapping of a dielectric plastic film to coat the electrodes. For precise and programmable printing of the patterned electrodes, we used a digital plotter with a ballpoint pen filled with a silver nanoparticle (AgNP) ink. Instead of using conventional material deposition methods, such as chemical vapor deposition, printing, and spin coating, for fabricating the thin dielectric layer, we used a simple method in which we prepared a thin dielectric layer using pre-made linear, low-density polyethylene (LLDPE) plastic (17-um thick) by simple wrapping. We then sealed it tightly with thin silicone oil layers so that it could be used as a DMF chip. Such a treated dielectric layer showed good electrowetting performance for a sessile drop without contact angle hysteresis under an applied voltage of less than 170 V. By using this straightforward fabrication method, we quickly and affordably fabricated a paper-based DMF chip and demonstrated the digital electrofluidic actuation and manipulation of drops.

Poster Presentation : **ELEC.P-453**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Unraveling Synergetic and Antagonistic Effects in the Rational Design of Ni- and Ru-Based Water Splitting Electrocatalysts

Filipe Marques Mota, Dong Ha Kim*

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

Tuning the bifunctional fingerprints of the hydrogen and oxygen evolution reactions (HER and OER) of water splitting electrocatalysts through the rational design of hybrid architectures incorporating multiple phases with precise functionalities is of increasing attention. Herein, Ni- and Ru-based electrocatalysts with increasing Ni/Ru content ratios were designed through a one-step heat treatment at 250°C of synthesized ruthenate nanosheets, and $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ and $\text{NaH}_2\text{PO}_2 \cdot \text{H}_2\text{O}$ precursors, under argon flow. A favored interaction between Ni ions and the negatively charged ruthenate surface directed an optimized in-situ growth of Ni_2P moieties with size below 5 nm. XPS measurements confirmed, however, that these narrow moieties were swiftly oxidized to NiO, whereas larger Ni-based agglomerates at higher Ni/Ru ratios were less prone to oxidation. This size-dependent propensity of Ni_2P moieties toward oxidation is reported here for the first time. Most importantly, at Ni/Ru=0.36 the incorporated NiO favored a superior OER performance with a 1.7-fold activity enhancement at limiting current densities. An antagonistic effect in the HER performance of these hybrid materials was, nonetheless, simultaneously observed and ascribed to the gradual incorporation of these oxide species on the surface of the Ru-based support. Our results reflect the difficulty in the integration of multiple phases during the synthesis procedure and the effect of an interaction between both materials on the resulting catalytic behavior.

Poster Presentation : **ELEC.P-454**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Incorporating excess lithium into LiMn₂O₄ via thermally induced grain fining: Promoted lithium-ion diffusion in Li-excess LiMn₂O₄

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Bionano Technology, Hanyang University, Korea

¹*Department of Bionano Technology, Hanyang University, Korea*

LiMn₂O₄ (LMO) is one of the famous cathode materials for a Lithium-Ion Batteries (LIBs) for its high power, low toxicity and cost. However, because oxidation number of Mn is easily changed, LMO shows a lower capacity and poor stability. Therefore, it is important to solve this problem by controlling the oxidation number of Mn. We suggest a facile method through annealing process in a reducing atmosphere for a high stable LMO. When Mn₂O₃ is reduced by NH₃, it becomes porous Mn₃O₄ with smaller grain size compared to conventional LMO (C-LMO). These pores contain more lithium inside, which results in Lithium-rich LMO (L-LMO). This L-LMO is highly stable attributed to its excess lithium source. The L-LMO also shows enhanced Li-ion diffusivity from additional fast dual Li-ion migration channels.

Poster Presentation : **ELEC.P-455**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

N-Doped Graphitic Carbon Coated Fe₂O₃ Using Dopamine as an Anode Material for Sodium-Ion Batteries

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Department of Chemistry, Dong-A University, Korea

Sodium ion batteries (SIBs) have attracted much attention for the application in large-scale energy storage systems (ESS) the next generation energy storage devices because they have the advantages of natural abundance and low cost. However, high-performance anode materials are still needed. Iron oxide (Fe₂O₃) is considered one of the promising anode materials because of its abundance, high theoretical capacity (about 1007.0 mAh g⁻¹), low cost, and non-toxicity. However, pristine Fe₂O₃ is accompanied by considerable volume change, causing electrode pulverization and agglomeration of Fe₂O₃ particles during charge-discharge processes. As a result, the pristine Fe₂O₃ undergoes relatively low reversible capacity and cycle stability. To overcome these problems, we synthesized Fe₂O₃ coated with N-doped graphitic carbon (Fe₂O₃/NGC) using dopamine as carbon and nitrogen sources. Compared with pristine Fe₂O₃, Fe₂O₃/NGC composite exhibited the improved reversible capacity of about 497.66 mA h g⁻¹ after 150 cycles at 100.7 mA g⁻¹ and 0.01-3.0 V.

Poster Presentation : **ELEC.P-456**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Study of electrocatalytic oxygen reduction reaction on metal nanocluster based electrodes

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The development of effective electrocatalysts for the oxygen reduction reaction (ORR) has caught much attention because it represents a critical cathodic reaction in fuel cells and other electrochemical energy devices. Despite extensive research progress, the commercialization of fuel cells has been hindered so far by the sluggish reaction dynamics and by the expensive platinum catalysts. Therefore, a number of studies have focused on non-platinum electrocatalysts. Recently, several studies have shown that gold nanoparticles increase ORR activities. In this study, The ORR activity of the nanostructure composed of metal nanocluster and carbon material was investigated, and effect of electrolyte basicity and metal doping effect of thiolate-protected nanoclusters were examined. First of all, mixture of Au₂₅ and multi-walled carbon nanotube(CNT) were cast on the glassy carbon electrode(GCE), then the fabricated GCE showed higher conductivity and efficiency on ORR. Next, the fabricated electrode made the onset potential of ORR shift more positive on the alkaline environment than neutral electrolyte condition. In addition, Ag₂₅ which has a lot of similarity with Au₂₅ in geometry exhibited improved ORR activity. In conclusion, electrocatalytic activity of ORR could be adjusted using modification of metal atom, pH and addition of carbon material. These ways to change the catalytic effect might help the design of tailored catalysts for the other electrocatalytic reactions.

Poster Presentation : **ELEC.P-457**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Thermally Induced Nanostructuring for the Synthesis of Core/Shell Structured CoO/CoS_x Electrocatalyst

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Typically, a high surface area of an electrocatalyst is required for a strong catalytic activity in dye-sensitized solar cells (DSSCs). For this reason, numerous bottom-up nanostructuring strategies were proposed to increase the surface area of cobalt compounds (CoO_x, CoS_x) as an alternative to platinum electrode. However, they are prone to structural collapse during sulfide treatment at high temperature. Therefore, a rational synthesis is needed to fully accommodate the porosity and the surface chemistries of the sulfide-treated cobalt compounds. In this work, we synthesized porous Core/Shell CoO/CoS_x from solid sphere-shaped Co₃O₄ via simple two-step top-down method. Co₃O₄ is reduced in ammonia condition generating mesoporosity inside the particle from structure rearrangement. After that, CoS_x shell is formed by sulfide thermal treatment while porous CoO core is maintained inside. This unique Core/Shell matrix enhances catalytic activity (from high surface area of CoO) and also makes faster charge transfer reaction (from CoS_x) as a comparable electrocatalyst to platinum in DSSCs.

Poster Presentation : **ELEC.P-458**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Non-enzyme biosensor using nickel particles immobilized indium tin oxide electrodes for selective detection of uric acid

Chang Jun Lee, Won-Yong Jeon, Young Bong Choi^{*}, Hyug-Han Kim^{*}

Department of Chemistry, Dankook University, Korea

There was uric acid that act as a bio-marker to detect gout. In biosensor using electrochemical methods, uric acid was difficult to selectively detect due to oxidation reaction by other interfering substances. In addition, there was disadvantage that the enzyme was expensive to use. However, selective quantitative analysis of uric acid was possible at low cost by using nickel particles. First, the polymer, polyvinylimidazole(PVI), is immobilized on the indium tin oxide (ITO) electrode using the electrodeposition method, and then the nickel solution was adsorbed by PVI. After washing modified electrodes, the solution with uric acid was then raised to react with nickel. Finally, modified electrodes was washed once more to remove unattached uric acid with nickel. The electrodes was confirmed through SEM and EDS for morphology and presence of nickel. The electrochemical impedance spectroscopy(EIS) for each substance carried out on the electrode based the changed resistance. Through differential pulse voltammetry(DPV), we plotted the calibration curve for quantitative analysis of uric acid and checked the effect of interference substances in human body such as ascorbic acid, dopamine, and glucose. As a result, this study was showed in the possibility of a biosensor capable of selectively detecting uric acid.

Poster Presentation : **ELEC.P-459**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Reductant-free synthesis of carbon dots-supported Ag-Cu catalysts for electrocatalytic oxygen reduction reaction

Hoseop Im, Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Carbon dots (CDs, also referred to in some literature as carbon quantum dots) have emerged as an important class of active nanomaterials for a variety of purposes and applications. For the use of optical energy conversion and related fields, there has been extensive research on their electron transfer process and photoinduced charge separation. However, as an excellent electron acceptor and electron donor, carbon nanoparticles have promising potential to be an oxidizing or reducing agent, which have rarely been reported. In this presentation, carbon dots-supported silver-copper (Ag-Cu/CDs) was prepared by using CDs as reducing agent. The prepared Ag-Cu/CDs didn't show any color change or aggregation for more than one month. This result indicated that the CDs were weak stabilizing agents to keep Ag-Cu nanoparticles from aggregation. To the best of our knowledge, the use of CDs as reducing and stabilizing agents has rarely been reported in conjunction with their use in the fabrication of metallic nanoparticles. The electrocatalytic activity of the Ag-Cu/CDs for oxygen reduction reaction in alkaline media was investigated by rotating disk electrode, rotating ring-disk electrode, and cyclic voltammetry. Indeed, the resultant Ag-Cu/CDs composites exhibited good catalytic activity for the reduction of oxygen, compared with the individual Ag (or Cu) nanoparticles synthesized by citrate reduction. The compositional/structural features are characterized by high-resolution transmission electron microscopy, Fourier transform infrared and UV-Vis spectroscopy, and X-ray diffraction. 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-460**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Synthesis and characterization of cobalt-iron composites for electrochemical water splitting

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The electrochemical water splitting has long been considered a promising approach to producing clean hydrogen fuel using renewable energy sources. The hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are the major half reactions occurring in the cathode and the anode respectively in the electrochemical water splitting reaction. At present, IrO_2 (or RuO_2) and its compound materials are the most traditional anodic activity catalysts for OER. However, precious materials have disadvantages, such as high cost, scarce resources and inferior durability, which impede their widespread commercialization and limit their performance. Therefore, there is an urgent need to search for new cheap metal catalysts with unexceptionable electrocatalytic properties for OER. Herein, we present the synthesis and characterization of nanostructured cobalt-iron composites (Co-Fe) that exhibit catalytic activity comparable to those of the state-of-the-art nonprecious catalysts. The catalysts are fabricated from inexpensive cobalt and iron precursors through a corrosion strategy without any additional agents, such as reductants. The Co-Fe catalysts are characterized by X-ray diffraction, transmission electron microscopy, and scanning electron microscopy. We also investigate the electrocatalytic activity of the Co-Fe catalysts for OER and compare them with commercial carbon-supported iridium. 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-461**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Fabrication of an Electrochemical Dual Microsensor for Simultaneous Monitoring of Hydrogen Sulfide and Oxygen

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A gas transmitter hydrogen sulfide (H₂S) is recognized as an important neuronal messenger in brain. Oxygen (O₂) is vital to most living organisms and a direct indicator especially under hypoxia condition. Thus, proper tools capable of measuring both H₂S and O₂ at the same time would allow us to investigate the interrelated dynamics between H₂S and O₂ in various biological systems. In this study, the development of an amperometric microsensor for real-time simultaneous measurements of H₂S and O₂ is demonstrated. 50 μm Pt wire and 25 μm Pt wire are individually embedded in a theta glass capillary and compose working electrodes. The ends of both Pt wires are electrochemically etched, and each Pt micropore is filled with different metal nanoparticles via electrodeposition. Then, the H₂S sensing electrode is coated with an electropolymerized thin film. On the other hand, a gas permeable membrane which gives silane modification is dispersed over the surface of the O₂ sensing electrode. Each electrode is finally optimized by determining a proper potential for sensing its target gas molecule only. The analytical performances of the developed dual sensor are verified in terms of the bioavailability. 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-462**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Electrospun Iridium Nanotubes for Carbon Monoxide Oxidation Reaction

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In these days, carbon monoxide (CO) is a universal poisonous air pollutant. As a cleaning method for this toxic gas, electrochemical oxidation of CO to carbon dioxide (CO₂), in some cases with water assistance, using active electrocatalysts is continually studied. Precious metals, such as Pt and Pd, are well-known complete oxidation catalysts with good activity and stability. Meanwhile, iridium and iridium oxide are also studied in various ways. However, there is still lack on research of CO oxidation with Ir. In this work, metallic iridium nanotubes are synthesized by electrospinning, heat-treatment (calcination) and additional reduction process. We examine the morphologies of the prepared iridium nanotubes by field-emission scanning electron microscopy (FE-SEM) and confirm the reduction of iridium oxide nanotubes to the metallic Ir counter part by X-ray diffraction (XRD). Electrochemical activity for CO oxidation is measured by cyclic voltammetry and amperometric i-t curve in 0.5 M H₂SO₄ aqueous solution containing 0.03 M NaCl. Conclusively, metallic iridium nanotubes show a good sensitivity for CO oxidation. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2017R1A2A2A14001137).

Poster Presentation : **ELEC.P-463**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Photoelectrochemical properties of Cuprous Oxide Nanowire

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Cu₂O is a p-type semiconductor material and possesses a variety of advantages for the application of photoelectrochemical(PEC) water splitting. In particular, the electronic bandgap of 2.1 eV can promote the absorption toward the visible light and from the earth abundant materials, the developing cost of Cu₂O is relative low. Relative to the oxygen evolution reaction of PEC water splitting, the hydrogen evolution reaction has been rarely examined due to the scarcity and instability of the materials. In this research, we developed p-type 1-dimensional Cu₂O nanowires by the electrochemical anodization and post-thermal treatment. For the fabrication of Cu₂O nanowires, the copper plate was cut with 2 x 2.5 cm², subsequently polished using the sandpaper and finally, immersed in 1 M HCl solution. After cleaning with D.I water, Cu(OH)₂ was fabricated by electrochemical anodization in 1 M NaOH solution. In order to transform blue colored Cu(OH)₂ to yellow-colored Cu₂O, the Cu(OH)₂ was annealed in tube furnace at 350 oC under Ar gas for 4h. Furthermore, one more thermal treatment at 550 oC under Ar gas for 1h was performed to improve the crystallinity of Cu₂O film under no significant modification of the morphology. At this time, the Cu₂O film exists in the orange-colored state. After that, photocatalyst is coated in Cu₂O. More detail analyses such as FE-SEM, XRD and PEC performance would be presented.

Poster Presentation : **ELEC.P-464**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Colorless-to-neutral gray electrochromic devices fabricated with inorganic nanocomposite films

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A nanocomposite NiO film was prepared on PET/ITO by simple wet coating method. The electrochromic properties of NiO electrode investigated in none-aqueous lithium electrolyte(0.1M LiClO₄/PC) by means of optical transmittance, cyclic voltammetry and chronoamperometry measurements. The nanocomposite NiO film shows a excellent electrochromic performance with a variation of transmittance up to 36.6% at 660 nm and exhibits good response time for oxidation and reduction.(8.3s, 10.1s)The nanocomposite NiO and WO₃ thin film were combined to fabricate complementary electrochromic device, which showed an optical modulation of 50% at 660nm and was very stable up to 1,000 cycles in lithium gel electrolyte.

Poster Presentation : **ELEC.P-465**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Atomic-scale combination of germanium-zinc distorted array for structural and electrochemical evolution

Gyujin Song, Soojin Park^{1,*}

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Alloy materials have been emerged to achieve compatible properties in various applications. The structural manipulation, however, requires sensitive and complicated synthetic process. Herein, we report atomic-scale combination of germanium-zinc distorted alloy exhibiting uncertain eutectic point in a phase diagram can imply a great potential to form atomically collaborated array via a simple fabrication method. When interconnected together, it prevents a fatal sublimation of germanium/germanium oxide during gas-solid phase reduction reaction and allows outstanding electronic conductivity as well as high available capacity in lithium-ion batteries, leading to structural and electrochemical evolution of germanium/zinc distorted array. Further, the unique features are clearly confirmed through in situ analysis.

Poster Presentation : **ELEC.P-466**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Rapid determination of norovirus using electrochemical nanobiosensor via WS₂ nanoflower-bioreceptor hybrid

Seung Hoon Back, ChanYeong Park¹, Tae Jung Park*

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Norovirus is one of the infectious diseases in the world by eating raw foods which were infected by others, and there are many people could be infected to touch and to eat contaminated things easily. Thus, it is important to develop highly sensitive and selective diagnosis tools of detection for norovirus are needed. So far, there are myriad types of detection methods were studied for the virus, among them, we have focused on the electrochemical nanobio hybrid sensor for its sensitive and selective properties. In this work, we have studied nanomaterials and to develop their morphology. Extending to the 2D flat structure and 3D structure of flower-like shape materials (WS₂NFs) enhances their properties as a bio sensing platform due to their spacious surface area. In addition, the WS₂NFs were coated with AuNPs on their surface to improve the electrochemical properties and to provide the immobilization place with the peptides. The performance of the nanobio hybrid electrochemical sensor was tested by electrochemical impedance spectroscopy, and to result to a low detection limit (3.79 copies/mL) in real virus sample by extracted from an oyster. These results indicate that the nanobio hybrid sensor can be applied to various biosensing platforms for point-of-care testing. Moreover, the potential of biosensor based on 2D materials in cooperation with AuNPs for the norovirus detection was demonstrated by the experiment results.

Poster Presentation : **ELEC.P-467**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Anodic WO₃ Nanoporous Film for Solar Water Oxidation

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Nanoporous tungsten trioxide (WO₃) photoanodes are potential candidates for the anodic part of a solar water-splitting device that produces hydrogen fuel and oxygen from water. These nanoporous materials can improve performance in photooxidation reactions compared to nonporous materials because of enhancements in light scattering, increases in surface area, light absorption and carrier collection. To evaluate the presence of these effects and their contributions toward energy conversion efficiency, a variety of nanostructured WO₃ photoanodes were synthesized by anodization of tungsten foils. Films of nanoporous WO₃ platelets were grown via anodization of tungsten foil, the morphology of the films was controlled by the anodization conditions, and the current-voltage performance was studied. The observed photocurrents were consistent with the apparent morphologies of the nanostructured arrays. Measurements of electrochemically active surface area and other physical characteristics were correlated with observed differences in absorbance, external quantum yield, and photocurrent density for the anodized arrays. The capability to quantify these characteristics and relate them to photoanode performance can allow for selection of appropriate structural parameters when designing photoanodes for solar energy conversion. Keywords: Tungsten oxide, anodization, nanoporous, photooxidation, photoanode.

Poster Presentation : **ELEC.P-468**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Electrocatalytic activity of molybdenum oxide nanoparticles dispersed on 2,6-diaminopyridine functionalized reduced graphene toward dopamine detection in presence of ascorbic acid.

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We have reported the synthesis of a 2,6-diaminopyridine functionalized electrochemically reduced graphene supported MoO₃ (2,6 DAP-ERGO/MoO₃) nanocomposite by hydrothermal method and tested as an electro active catalyst for the detection of dopamine (DA) in presence of ascorbic acid (AA). The 2,6 DAP-ERGO/MoO₃ nanocomposite has been characterized by X-ray photoelectron spectroscopy (XPS) & field emission transmission electron microscopy (FE-TEM) technique. The electrochemical determination of dopamine was confirmed over the cyclic voltammetry (CV), Differential pulse voltammetry (DPV) in the presence of Ascorbic Acid at a high concentration as well as chronoamperometric (CA) experiment in a 0.1 M phosphate buffer solution (PBS) at pH 7.4. The impact of interference has been checked in being of several electro active biomolecules such as ascorbic acid (AA), serotonin (5-HT), glucose, Hydrazine (N₂H₄) and uric acid (UA). The 2,6 DAP-ERGO/MoO₃ modified electrode demonstrated an attractive electrochemical response with relatively better sensitivity (271.57 μ A mM⁻¹cm⁻²) a broad linear detection range (0.1 μ M - 900 μ M) & detection limit 0.142 μ M (S/N = 3). The diffusion coefficient for dopamine determination has been estimated as 4.6×10^{-8} cm² s⁻¹. The practical application of this proposed nanocomposite was analyzed using human urine sample which exhibited satisfactory result.

Poster Presentation : **ELEC.P-469**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Stretchable components design of lithium-ion battery toward wearable electronics

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With the steep progress of wearable electronics such as health care devices, soft electronics, and implantable devices, it is essential to develop energy-storage devices with high stretchability and reasonable electrical performance for powering wearable devices. To achieve the above stretchable energy-storage devices, especially batteries, lots of research have been focused on fabrication of a gel polymer electrolyte (GPE) that substitutes a conventional liquid electrolyte and separator because they can be stretched. However, this GPE suffer from sluggish ionic transport compared with conventional liquid electrolyte systems. Furthermore, they may induce short circuit problem under mechanical deformations. Thus, we propose the poly(styrene-*b*-butadiene-*b*-styrene) (SBS)-based stretchable separator, fabricated by using nonsolvent induced phase separation (NIPS) method. This stretchable separator membrane provides facile ion transport channels between two electrodes as well as prevents internal short circuit even under 270% strain. Likewise this separator, stretchable electrode based on conductive fillers/polymer composite, which provides both mechanical robustness (stretching/releasing 1000 cycles) and high electrical conductivity under a strain of 200%, is a core components in the stretchable energy-storage devices in the way. We fabricated the hybrid carbon/polymer (HCP) composite using elastic polymer, carbon nanotubes and carbon black in simple process which can effectively work as a stretchable current collector with providing an efficient electrical pathways. Finally, we achieve stretchable aqueous Li-ion batteries comprising as-prepared stretchable electrode and stretchable separator membrane.

Poster Presentation : **ELEC.P-470**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Chitosan-Based Polymer Electrolyte Containing Silver nanowire of Various Shapes

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Solid electrolytes have attracted enormous interest due to their wide applications in electrochemical devices such as sensors, and batteries. Solid electrolytes can be categorized into two different groups (ceramic or polymer electrolytes) depending on materials used. Ceramic electrolytes exhibit ionic conductivity higher than that of polymer electrolytes, however, brittle mechanical property of ceramic electrolytes is main obstacle for their easy application. In contrast, polymer electrolytes is flexible and can be easily applied to construct electrochemical devices, but their ionic conductivity is usually low. There have been numerous studies to increase ionic conductivity of polymer electrolytes by adding various plasticizers, and nanowires. To the best of our knowledge, nanowire's shape-dependence on ionic conductivity has not been studied. Herein, we synthesized silver nanowires of various shapes (sphere, wire, triangle) and used them as additives to enhance ionic conductivity of chitosan-based polymer electrolyte. References [1] S. N. Suraiya Begum, Ramanathaswamy Pandian, Vinod K. Aswal, Radha Perumal Ramasamu, Chitosan-Gold-Lithium Nanocomposites as Solid Polymer Electrolyte *Journal of Nanoscience and Nanotechnology* 2014 14, 1113 [2] Yun-Chae Jung, Myung-Soo Park, Chil-Hoon Doh, Dong-Won Kim, Organic-Inorganic Hybrid Solid Electrolytes for Solid-State Lithium Cells Operating at room Temperature *Electrochimica Acta* 2016 218, 271-277. [3] Agnieszka pawlicka, Marins Danczuk, Wladystaw Wieczorek, Ewa Zygadlo-Monikowska, Influence of plasticizer Typr on the properties of Polymer Electrolytes Based on Chitosan *J. Phys. Chem.* 2008 112, 8888-8895.

Poster Presentation : **ELEC.P-471**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Noticeable photocurrent generation through improved electrochemical communication between cyanobacteria and electrode

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There is a growing interest in using photosynthetic microorganisms for converting solar energy to electrical energy aiming at practical application. Despite extensive research using different microorganisms, however, existing methods have been suffered from limited photocurrent for that purpose. Here, we report that appreciable photocurrent could be generated in a photo-bioelectrochemical cell (PBEC) where cyanobacterium *Anabaena variabilis* (*A. variabilis*) was used as a photo-biocatalyst that oxidizes water by solar light to produce electrons. The PBEC was composed of reduced graphene oxide-coated indium tin oxide electrode, *A. variabilis*, and an electron mediator. When *A. variabilis* was dispersed in solution and 1,4-benzoquinone was used as a redox mediator, our PBEC produced appreciable photocurrent of 213 $\mu\text{A cm}^2$ at an applied potential of 0.4 V vs. Ag/AgCl, which is far greater than reported results, most of which use cyanobacterial biofilms on the electrode surface. The effects of mediator concentration and operating temperature on the photocurrent have also been examined. Methodology in this study could be extended to cover other cyanobacteria, electrode materials, and mediators to further enhance photocurrent. Our results demonstrate a possibility of utilizing cyanobacteria that are ubiquitous in environment as alternative energy sources.

Poster Presentation : **ELEC.P-472**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Exploration of Photo and Electrochemical Studies with an Efficient Electrocatalyst on BiVO₄ Photoelectrode for Photoelectrochemical Water Splitting.

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

Photoelectrochemical (PEC) water splitting to produce clean hydrogen provides a desirable approach to solving global environmental and energy problems. Bismuth vanadate (BiVO₄) has emerged as one of the most promising photoanode materials for oxidising water due to its visible light activity and low cost. However, BiVO₄ Photocatalyst has suffered by the slow charge separation kinetics at solid/electrode interface that limits the photoelectrochemical performance. In order to minimize the poor properties, we modified the BiVO₄ with effective electrocatalysts, which was investigated experimentally under light illumination. The subsequent addition of electrocatalysts as an effective Oxygen evolution catalyst subsequently reduces the large overpotential and generates higher photocurrent. The charge transfer properties of the photoelectrodes can be effectively tuned by controlling the electrocatalysts loaded, thereby optimizing PEC performance. Electrochemical impedance spectroscopy (EIS) evidenced that electrocatalysts deposition can substantially lower the charge transfer resistance (R_{ct}) at the semiconductor interface. Further, the advantages and drawbacks of catalyst deposition routes and the role of photoelectrochemical and advanced spectroscopic techniques for elucidation of the mechanism of the photocatalytic action will be discussed in detail.

Poster Presentation : **ELEC.P-473**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Analysis of Oxidizing occurrence of Single Nickel Nanoparticle for Urea Oxidation by Electrocatalytic method.

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The current detected by the collided single nanoparticle (NP) of Nickel (Ni) on a Platinum (Pt) ultramicroelectrode (UME) surface was detected by electrocatalytic amplification method. A linear increase of collision frequency and transient current signal as a function of time was detected by the Ni NP oxidized to Nickel oxide NP. The same results were detected when Ni NP was oxidized by purging oxygen gas for a period of time. The used electrochemical reaction was urea oxidation in alkaline solution because Ni has electrocatalyst characteristic for the urea oxidation in alkaline solution. The transient current signal detected by a single Ni NP on the Pt UME shows a staircase signal with involving slow signal decay. The applied potential and concentration of urea were optimized for increasing signal to noise ratio. The magnitude of current signal and signal frequency were analyzed. Through analysis of the electrocatalytic characteristic of single Ni NPs, this study offers insight toward their future application.

Poster Presentation : **ELEC.P-474**

Electrochemistry

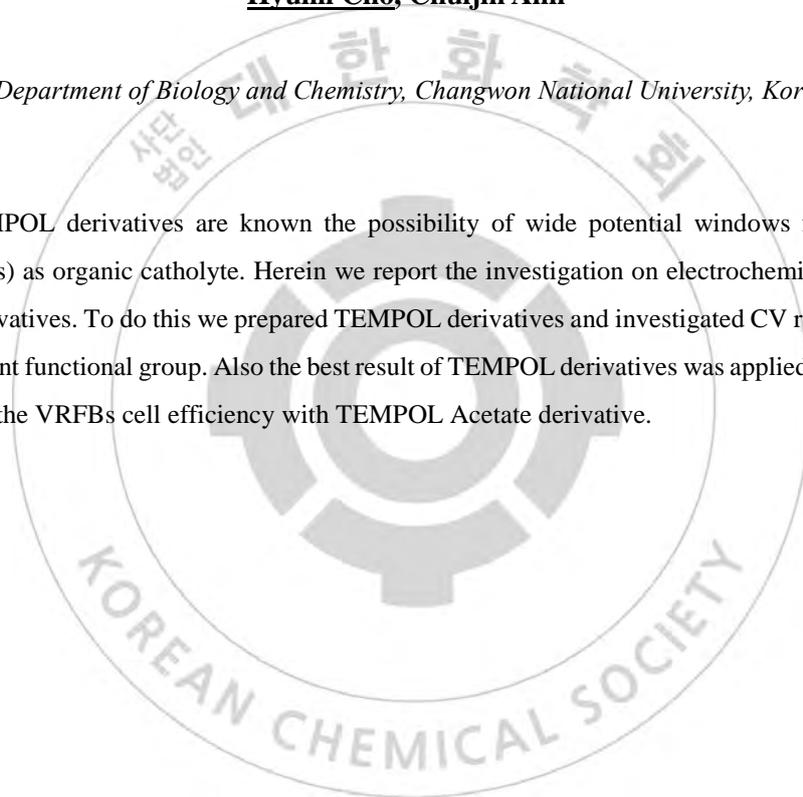
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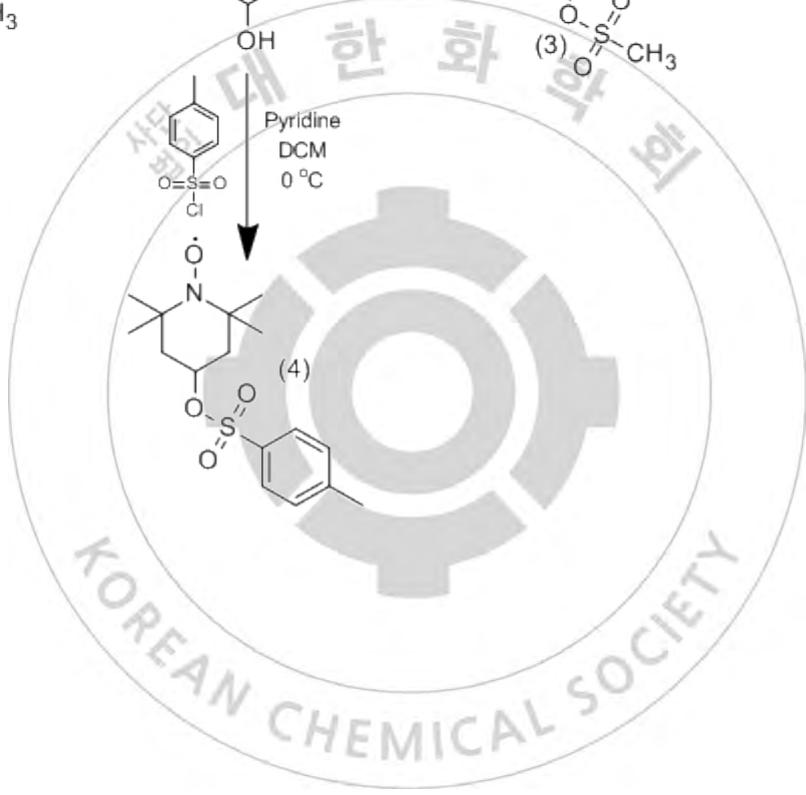
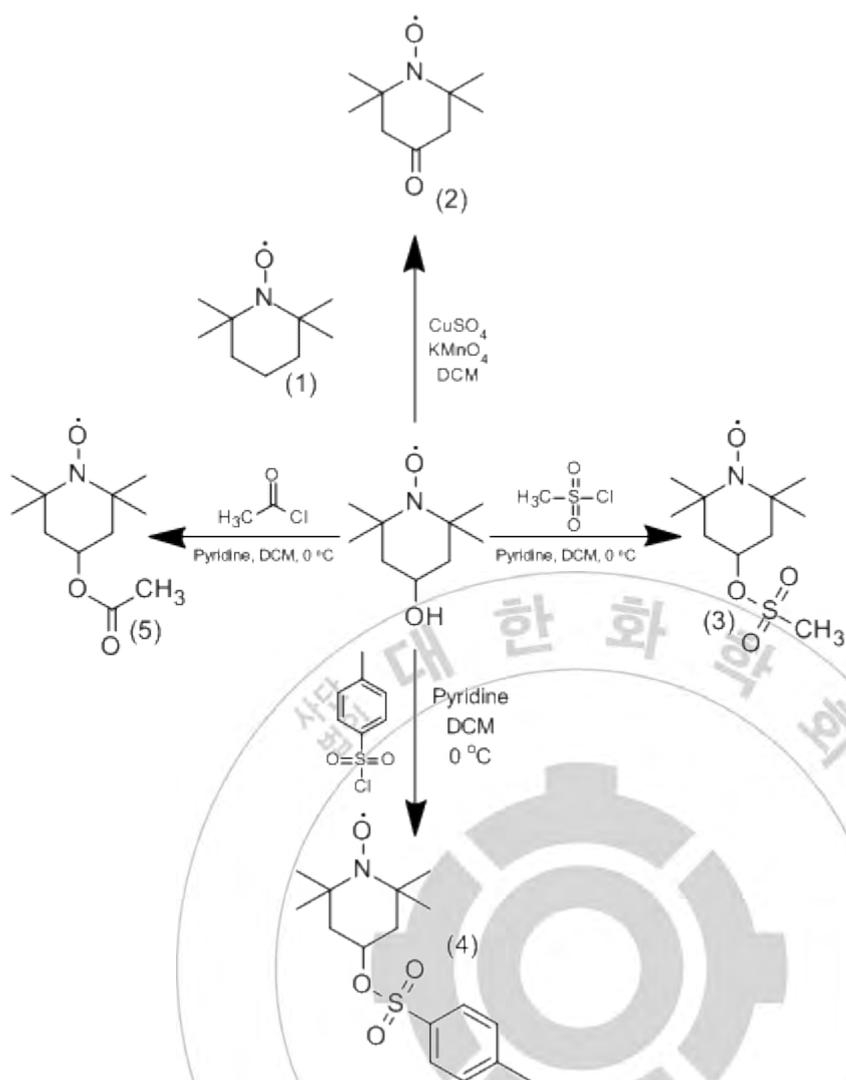
Preparation and Electrochemical Investigation of TEMPOL Derivatives : Apply to Redox Flow Battery

Hyunil Cho, Chuljin 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-475**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Pt and Ru electrocatalysts using the synergistic effect of single atoms and nanoparticles for high hydrogen evolution

Siraj Sultan, Ahmad Mosen Harzandi, Kwang Soo Kim*

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

Hydrogen has been considered as a clean renewable energy system. Pt has been the universal choice for the acidic hydrogen evolution reaction (HER), $2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2\uparrow$, because Pt displays a much lower overpotential and higher current density than other materials. For cost efficiency, the development of non-precious materials has also been in progress, but yet Pt is still the universal choice. Also, milligram Pt loadings for a high HER activity are being developed, but an $\sim 1\mu\text{g}$ loading for an inexpensive and highly efficient hydrogen production has not yet been realized. Herein we adopt an atomic-scale engineering strategy for Pt-based catalysts with the controlled deposition of Cu, Fe and Co atoms onto/into graphitic tubes (GTs). This has led us to develop the HER catalyst in which GTs encapsulate FeCo alloy nanoparticles (NPs) with an ultrathin Cu layer inside the tube wall and have single Pt atoms embedded at the GT outlayer and nanosized Pt clusters on the tube surface. The catalyst with only $1.4\mu\text{g}$ of Pt (per electrode area (cm^2)) loading is found to exhibit a superior HER activity with a very high turnover frequency (TOF) and both a small overpotential and stability. With a 1/80th Pt loading of a commercial 20% Pt/C catalyst, in 0.5 M H_2SO_4 the catalyst achieves a current density of 10 mA cm^{-2} at an overpotential of 18 mV, and shows a turnover frequency of 7.22 s^{-1} (96 times higher than that of the Pt/C catalyst) and long-term durability (10,000 cycles). The catalytic activity is enhanced due to the synergistic effect between the Pt clusters and single Pt atoms [J. N. Tiwari et al. Nature Energy 3, 773-782 (2018)]. A similar work on Ru clusters and single atoms is also discussed [J. N. Tiwari et al. (submitted); A. M. Harzandi et al. (submitted)].

Poster Presentation : **ELEC.P-476**

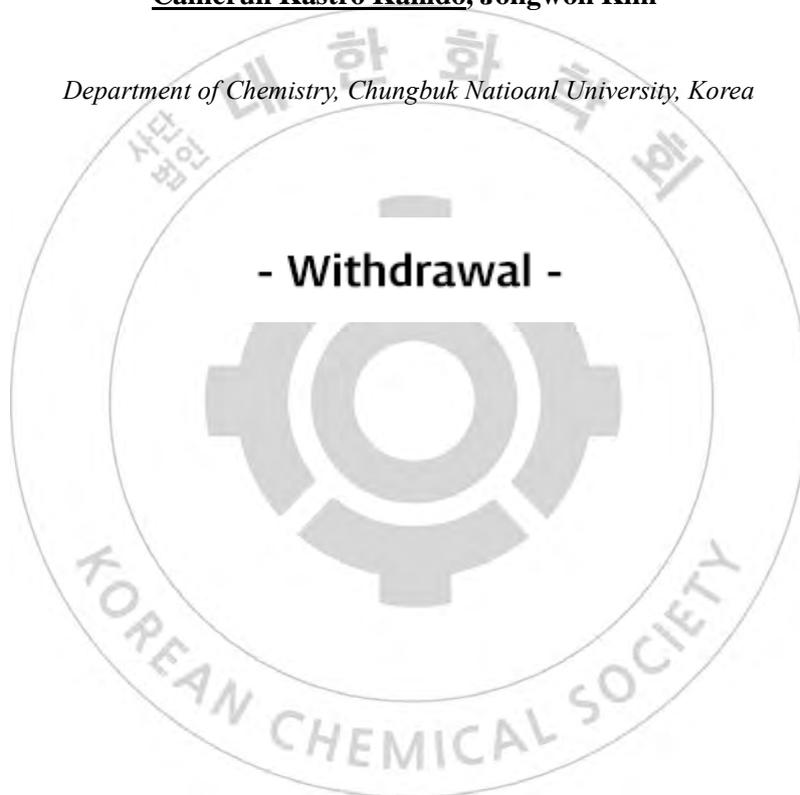
Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

[Withdrawal] Comparative Study of the Effects of Nanostructures of Au on the Electrochemical detection of As

Camerun Kastro Kanido, Jongwon Kim*

Department of Chemistry, Chungbuk National University, Korea



Poster Presentation : **ELEC.P-477**

Electrochemistry

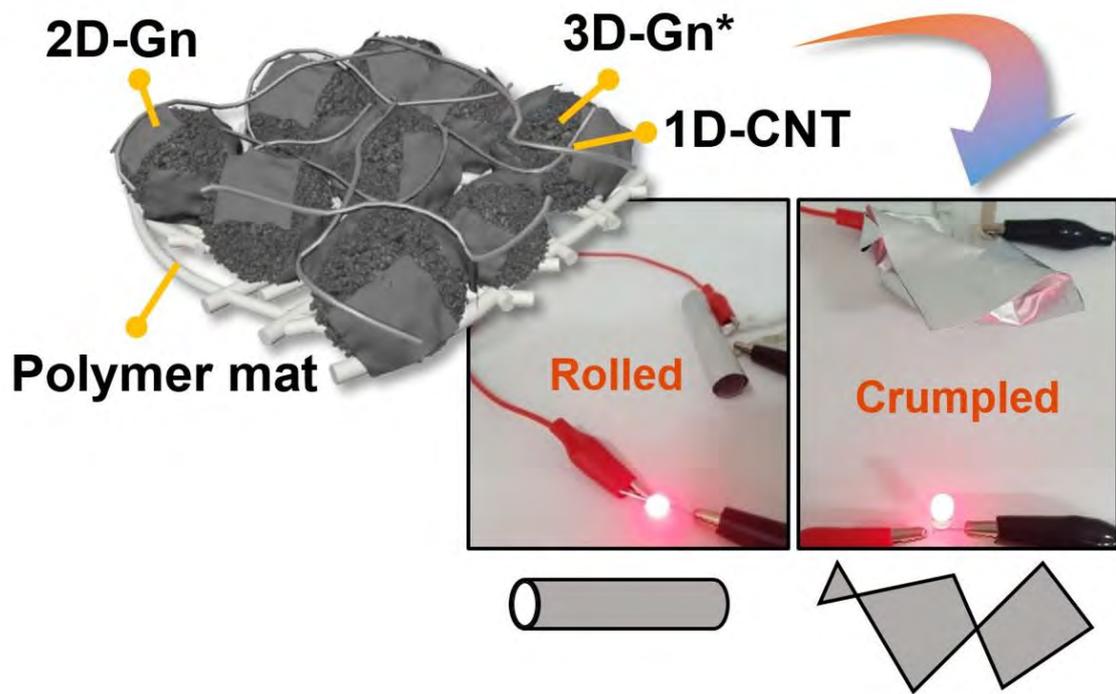
Exhibition Hall 2, THU 11:00~12:30

A Hierarchically Structured Multi-dimensional Carbon Composite Anchored to Polymer Mat for Super-flexible Supercapacitor

MyungJun Kwak

Ulsan National Institute of Science and Technology, Korea

A carbon electrode was designed to guarantee the flexibility of symmetric electric double layer capacitors (EDLCs) based on its architecture. Three different dimensional carbon materials were combined to achieve flexibility without sacrificing high performances: highly capacitive but poorly-conductive three-dimensional graphene (3D-Gn*) as a platform for electric double layer formation, one-dimensional carbon nanotube (1D-CNT) as an electrically conductive highway and two dimensional graphene (2D-Gn) for facilitating electron communications between 3D-Gn* and 1D-CNT. From a mechanical standpoint, the 1D-CNT provided an intertangled framework to integrate the main active material 3D-Gn* and anchored the active layer to a flexible polymer matrix. Resultantly, the symmetric EDLC based on the hierarchically structured multi-dimensional carbon electrodes anchored to flexible substrates was operated successfully at 3 V, ensuring high energy densities even under repetitive mechanical stress conditions.



Poster Presentation : **ELEC.P-478**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

In situ growth of polyaniline nanowires on interconnected porous carbon nanosheets for high-performance supercapacitors

Xuanzhen Jin, Yuanzhe Piao*

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Many kinds of conducting polymers have been extensively studied as electrode materials for pseudocapacitors. Among them, polyaniline (PANI) possesses high theoretical specific capacitance and is light weight and inexpensive. However, poor cycle stability of PANI restricts its real applications in commercial supercapacitors. Preparation of nano-PANI composited with nanostructured carbon materials such as activated carbon, carbon nanotubes and graphene is one of efficacious strategies to improve the electrode performance. Recently, 3D interconnected porous carbon (IPC) materials obtained directly from pyrolysis of potassium citrate salt were considered as promising new carbon substrates for energy devices. In this work, 3D IPC/PANI nanocomposites were prepared via a simple in situ growth of vertically aligned PANI nanowires arrays on IPC. The nanocomposites show excellent specific capacitance of 512 F·g⁻¹ at a discharge current density of 1 A·g⁻¹. In addition, the as-assembled asymmetric supercapacitor based on the nanocomposites also exhibits good capacitive properties and long-term cycling stability of 91% after 3000 cycles at 5 A·g⁻¹. The improved electrochemical performance of IPC/PANI is attributed to three factors: (1) highly interconnected 3D porous structure of the PC substrate which is beneficial for fast ion diffusion and shortening the transport distance of electrolyte ions in the charge/discharge processes; (2) stable IPC template of the composites which prevents swelling and shrinkage of PANI during the electrochemical redox processes; (3) ordered nanowire arrays of PANI which provide more active sites than random structured PANI.

Poster Presentation : **ELEC.P-479**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation of highly porous fluorine-doped CoFe₂O₄/graphene sheet nanocomposites for hybrid supercapacitors

Juhyung Choi, Yuanzhe Piao^{1,*}

Seoul National University, Korea

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A common approach to achieve enhanced performance of electrochemical energy device involves improving the charge transfer properties and optimizing the material structure. In this work, highly porous fluorine-doped CoFe₂O₄ sphere/graphene nanocomposites are prepared by one-pot facile hydrothermal method based on the Ostwald ripening mechanism. Incorporation of fluorine in CoFe₂O₄/Graphene improves charge transfer in the electrode material and ion diffusion by forming a porous structure that serves as an electrolyte reservoir during the redox reactions. The effect of the fluorine concentration on the nanostructural formation during the hydrothermal process is systemically studied. The fluorine-doped CoFe₂O₄/Graphene composite exhibits a high specific capacity of 288 C g⁻¹ (at a current density of 10 A g⁻¹). A hybrid supercapacitor based on the FS-CoFe₂O₄/GS composite exhibits a high energy density of 28.4Wh kg⁻¹ (at a power density of 0.9 kWkg⁻¹) at 1.6 V and a high capacity retention of 90% after 20,000 cycles.

Poster Presentation : **ELEC.P-480**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Facile synthesis of nickel cobalt hydroxide nanoneedle/graphene hydrogel composite as a binder-free electrode for asymmetric supercapacitor

Jeongmin Kang, Yuanzhe Piao*

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

Nickel cobalt hydroxide nanoneedle/graphene hydrogel nanocomposite is prepared by using a facile two-step method and further explored as a binder-free electrode for asymmetric supercapacitor. First, freestanding graphene hydrogel is prepared at low temperature using mild reducing agent. Second, nickel cobalt hydroxide nanoneedles are embedded in the graphene hydrogel by using hydrothermal method. Hydrophilic functional groups in graphene hydrogel make nickel cobalt hydroxide nanoneedles to be well-dispersed on the graphene nanosheet surface. Additionally, the freestanding property of graphene hydrogel is used to prepare a binder-free electrode, which can improve the energy density of the final generated asymmetric supercapacitors. The nanocomposite shows an excellent capacity of 544 C g^{-1} at 2 A g^{-1} in a three-electrode system. Moreover, the binder-free asymmetric supercapacitor achieves excellent performance with an energy density of 32.74 Wh kg^{-1} at a power density of 320 W kg^{-1} and good cycling stability with 85% capacitance retention at a current density of 10 mA cm^{-2} after 5,000 cycles. These excellent electrochemical performances are attributed to the synergistic effects of (1) high redox active material of nickel cobalt hydroxide, (2) hydrophilic functional group in graphene hydrogel for stable growth of nickel cobalt hydroxide, and (3) fast ion transport by the 3D porous network structure of graphene hydrogel. It is expected that the preparation strategy shown in this work can be used to fabricate other 3D structured nanocomposite for related energy devices.

Poster Presentation : **ELEC.P-481**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Formation of various metal oxide nanostructures by anodization in a hot glycerol electrolytes

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Anodic formation of metal oxide on the metal substrates have been use in various industrial fields to improve of corrosion resistance, heat insulation, anti-reflecting and decorate metal surface. Furthermore, anodization methods allows to formation of metal oxide nanostructure with one or three dimensionally. The anodic oxide nanostructures also have various advantages due to its high specific surface areas, high electron conductivity with vertically aligned geometry. For these reasons, anodization have been studied in several decades. To form anodic metal oxides, several parameters are concerned such as composition of electrolytes, applied potential or current, and reaction temperatures. In general, porous anodic Al₂O₃ are formed in acidic electrolytes, anodic TiO₂ nanotubes are formed in fluorine containing electrolytes at room temperatures. In this presentation, we introduce new anodization approach which is carried out in phosphate contained glycerol electrolyte at high temperatures. The anodization methods are easy to control chemical etching rate which leads to allowing unusual metal oxide formation and nanostructuring of Al, Ni and stainless steel.

Poster Presentation : **ELEC.P-482**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Enhanced Electrochemical Performances of Multiple Heteroatom Doped Carbon Nanocomposites for Supercapacitors

Dae Kyom Kim, Yuanzhe Piao*

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To meet the challenge of enhancement of energy density for electrochemical double layer capacitors, single heteroatom doping such as nitrogen doped carbon nanocomposite has been widely researched because of its abundance and facile synthesis process. To further improve the energy density of carbon electrode materials for capacitor, functionalization of carbon materials with multiple-heteroatoms have been studied recently. In this work, multiple heteroatoms such as N, F, and B as doping sources were introduced in the carbon nanostructure to induce higher synergistic effects. Fluorinated polyamic acid and boric acid were used as a doped source and multiple heteroatom doped carbon nanocomposites were obtained by calcination process at high temperature. The as-prepared samples were systematically characterized by SEM, XPS, and Raman spectroscopy. Also, the synthesized carbon materials exhibited higher specific capacitance and higher rate capability than single nitrogen doped carbon.

Poster Presentation : **ELEC.P-483**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Formation and Crystallization of Anodic Vanadium Oxide Nanostructures

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Over the past decades, transition metal oxides have been intensively studied due to their outstanding performance for photocatalysis, pollutant degradation and, biomaterials, etc. Among several types of metal oxides, Vanadium oxides have been considered promising materials in the fields of ion insertion, magnetic and electronics. In order to enhance the properties, one-dimensional nanostructures have been considered. A straightforward approach for the one-deimensional nanostrcutres is a self-organizing andoziation of metal substrate in a fluoride containing electrolytes. However, anodization of vanadium metals are quite challenge due to its fast dissolution rate during reaction. Moreover, formed vanadium nanostructures are required further crystallization for suitable applications. In this presentation, we will discuss about critical parameters for formation of anodic vanadium nanostructures and crystallization.

Poster Presentation : **ELEC.P-484**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Electrodeposition of Fe₂O₃ on modified FTO glass for efficient photoelectrochemical water splitting

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¹School of Nano & Materials Science and Engineering, Kyungpook National University, Korea

Fe₂O₃ has been extensively investigated as a promising materials for photoelectrochemical water splitting due to its 2.2 eV of favourable band gap, chemical and physical stabilities, abundant, and low cost. However, the reported efficiencies of water splitting are relatively lower than theoretically predicted value, mainly because of the extremely short life time of photogenerated charge carriers' and diffusion length, inert oxygen evolution reaction, and low flat band potential. In order to enhance the efficiency, various approaches are considered such as nanostructuring, doping, and co-catalysis. Particularly, for nanostructuring various approaches are used like hydrothermal, sol-gel, and electro deposition. Here, we are focused on formation of Fe₂O₃ nanostructures by electrodeposition on nano patterned fluorine-doped tin oxide (FTO) glasses. In order to achieve, porous FTO structures were formed by electrochemical etching before Fe₂O₃ deposition. Finally, we studied about the relationship between physical properties of porous FTO and photoelectrochemical efficiency.

Poster Presentation : **ELEC.P-485**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Structure preserving transformation of zeolitic imidazolate frameworks into polyhedral shaped hollow Co-B-O@Co₃O₄ catalysts for oxygen evolution reaction

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

Designing highly efficient and low-cost electrocatalysts for oxygen evolution reaction is required to promote the overall water splitting reaction. In this work, polyhedral shaped hollow cobalt-borate modified cobalt oxide composite (denoted as Co-B-O@Co₃O₄) electrocatalysts are successfully synthesized via calcination of ZIF-67 followed by NaBH₄ treatment. The prepared Co-B-O@Co₃O₄ catalysts maintain well unique polyhedral morphology of ZIF-67 after the NaBH₄ treatment. The unique polyherdral shaped hollow structure can effectively expose more active sites and enhance the mass transport. In addition, the introduced boron can tune the electronic structure and consequently improve the charge transfer of the catalysts. Benefiting from the above properties, the synthesized Co-B-O@Co₃O₄ catalysts show high catalytic activity and long-term stability for OER in alkaline solution. We further studied the catalytic performance of Co-B-O@Co₃O₄ in neutral pH environment. Our research can give perspective of catalyst tuning method to improve the overall catalytic performance while preserving its original structure simultaneously.

Poster Presentation : **ELEC.P-486**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Ultrafine Sn Nanoparticles Loaded on Structurally Well-designed Carbon Frameworks for High-performance Lithium Ion Batteries

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Lithium-ion batteries (LIBs) have been widely used as energy storage devices for mobile electronic devices and electric vehicles. Sn-based materials have been considered as a promising anode material for high performance of LIBs because of their appropriate working voltage, abundance, high theoretical capacity (992 mAh g⁻¹), and high electrical conductivity. However, Sn nanoparticles have some drawbacks such as capacity fading during the charge/discharge process due to aggregation and critical volume change (~300%). In this work, ultrafine Sn nanoparticles were loaded on structurally well-designed nitrogen- and phosphorus-doped hollow carbon framework and studied as an anode material for LIBs. The hollow structure of carbon can provide a void space to accommodate the volume expansion of the Sn nanoparticles and prevents the electrode from pulverization during the charge/discharge process. Also, the doping elements such as nitrogen and phosphorus in hollow carbon framework stabilize the electrochemical performance. Furthermore, the hollow carbon structures are widely interconnected by graphene which enables rapid electron and lithium ion transport to enhance rate and cycle performance. Consequently, the as-prepared Sn-hollow carbon nanocomposite exhibits excellent cycling performance even at a high current density of 1.0 A g⁻¹ (specific capacity of 1048 mA h g⁻¹ after 1000 cycles).

Poster Presentation : **ELEC.P-487**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Impregnation of Sn/SnO_x in uniform-sized hollow carbon spheres anchored graphene nanosheet as anode material for lithium-ion batteries

Taejin Hwang, Yuanzhe Piao*

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To meet the ever increasing market demands of higher capacity and energy density of Lithium-ion battery, many kinds of new electrode materials have been extensively studied recently. Among them, Sn-based materials have been widely studied as a promising candidate as anode material for Lithium-ion battery due to their high theoretical capacity and low cost. In this work, uniform-sized hollow carbon spheres of ~20 nm anchored on graphene nanosheet were synthesized via a facile and scalable process. Then, Sn/SnO_x was impregnated in the carbon nanostructure by a typical melt-diffusion process. The electrode prepared by using the as-prepared nanomaterial delivers a high rate capability of 290.0 mA h g⁻¹ at current density of 3 A g⁻¹ and good cyclability of 284.1 mA h g⁻¹ after 1000 cycles at 1 A g⁻¹. The excellent electrochemical performance is attributed to the uniform-sized hollow carbon spheres, which mitigates the volume expansion of Sn as physical barrier and enables Li-ions or electrons to easily move by improving electrical conductivity during discharge/charge process. Thus, the Sn/SnO_x impregnated nanocomposite is expected to be a promising anode material for lithium-ion batteries.

Poster Presentation : **ELEC.P-488**

Electrochemistry

Exhibition Hall 2, THU 11:00~12:30

Preparation of few-layered and vertically aligned MoS₂ by employing 3D interconnected porous carbon for electrochemical hydrogen evolution

Dongjin Ko, Yuanzhe Piao*

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

MoS₂ has emerged as a promising noble-metal-free electrocatalyst for electrochemical hydrogen evolution reaction. However, the catalytic performance of MoS₂ is limited by the low density of active sites. Reducing the layers and sizes of MoS₂ nanosheets and vertically aligning them on the conductive substrate are effective ways to increase the exposure of active sites for hydrogen evolution. However, decreasing number of layers and sizes of MoS₂ nanosheets have been problematic due to thermodynamic driving force. In this work, few-layered and small sized MoS₂ nanosheets were prepared by using interconnected porous carbon nanosheets as substrates. Experimental results show that the micropores can play an important role in growing few-layered MoS₂ on the carbon substrate. As an electrocatalyst for HER, the optimized MoS₂/IPC-2 composite exhibited a high catalytic activity (current density of 225 mAcm⁻² at -250 mV vs. RHE, and Tafel slope of 38mV/dec) and maintained steady performance for several hours of continuous HER test. Since the procedure is cost-effective and scalable, our method of preparing few-layered MoS₂ on porous carbon shows great potential as a competitive electrocatalysts for HER.

Poster Presentation : **EDU.P-489**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

What do the Pre-service Teachers Learn from the Overseas Educational Volunteer Activity?

JaeYoung Han

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National Institute for International Education has supported the Korean pre-service teachers to go abroad for the overseas educational volunteer activity since 2016. The pre-service teachers of Chungbuk National University went to Nicaragua and taught elementary and secondary students. They had to select the lesson, make the textbook, write a script in Spanish, prepare educational materials, and demonstrate teaching before going to Nicaragua. In Nicaragua they had to teach students, modify lesson and script, develop their teaching skills, and evaluate lessons. When they came back to Korea, they had to reflect on their overseas educational volunteer activity. In all of these procedures, the pre-service teachers learned a lot of things. The purpose of this study is to analyze the learning of pre-service teachers. The raw data is the pre-service teachers' (N=17) final reports. The learning was classified in three categories of preparation, teaching, and reflection. In the preparation, for example, they learned how to plan a lesson according to the context of the foreign country and to the level of students. In the teaching, for example, they learned how to interact with students and how to diversify the lessons. In the reflection, for example, they developed their own meaning of teaching. The overseas educational volunteer activity gave pre-service teachers very valuable experiences of true practicum. [This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2018S1A5A2A01036487)].

Poster Presentation : **EDU.P-490**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

Applying Systems Thinking For Depth Understanding of Scientific Model

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Learning the scientific model in classroom is to learn the thought of the scientist who discovered the model, but for decades science education has only presented the results of the discovered scientific model and hindered the true understanding of the model. This education can not be a sustainable education for the future. And genuine education about scientific models requires understand of process of model creation by scientists in terms of generation of models. It is not easy for students to understand this because most of the science models are feedback relationships that have an effect between elements rather than being explained by linear relationships of elements. Among the many models covered in the chemistry class, the Brönsted-Lowry model is the most reported that students have difficulty learning the model. In many countries these difficulties have been reported constantly, but it is still difficulties because of model's nature. Understanding the Brönsted-Lowry model requires a comprehensive understanding of the interaction of the various elements. It is the systems thinking to look at and explain the entire system from the mutually independent action of these various individual elements. This paper aims to enhance the understanding of the model by applying systems thinking to the Brönsted-Lowry model, which requires an explanation of the whole system through understanding the complex relationships of various factors. The results of this study are expected to provide a discussion on how to use systems thinking for sustainable chemistry education.

Poster Presentation : **EDU.P-491**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

A new high school integrated science new material part experiment research program

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Kangdong high school, Korea

The 2015 revised curriculum was applied in education part of South Korea. It is many change curriculum of high school integrated science subject. Specially, new materials part is changed about fourth industrial revolution. many high school integrated science curriculum text book was not activity of experiment about new material part. To solve the problem, We make a new experiment program using aniline and paper. this experiment program is simple. But, many students are easily understand about conductive polymer. As a result, students form interest about new materials part



Poster Presentation : **EDU.P-492**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

A Study on Effects of Class based on Science Practices on Cultivating Middle School Students' Science Core Competencies

Jeong Ah Choi*, Ae Ja Woo

General Science Education, Ewha Womans University, Korea

The Korean Ministry of Education (MOE) put an emphasis on science core competencies and suggested inquiry for developing core competencies in '2015 revised national science curriculum'. The class based on science practices is composed of eight practices, using the inquiry methods that scientists explore nature with, to not only help students be able to construct scientific concepts by themselves but also to cultivate core competencies. The purpose of this study is to see how students' perceptions about the cultivation of science core competencies are changing when applying a class based on science practices to first year middle school students. For this purpose, on the subjects of 42 students in the control group, a general science class was carried out in which teachers conveyed scientific knowledge. In the experimental group, the teachers conducted 27 science class sessions based on eight practices based class for 50 students. In both groups, a pre and post survey of science core competencies were conducted. More specifically, to understand the change in perception of competencies, a total of 20 students from the experimental group were interviewed in person. The result of this study is as follows. The overall science subjects' core competencies of experimental group students who experienced class based on science practices was significantly increased higher than that of the control group (p

Poster Presentation : **EDU.P-493**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

The Characteristics of Pre-service Science Teachers' Analogy Generating Processes

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In this study, we investigated the characteristics in the processes of generating analogy for lessons by pre-service science teachers. Eight pre-service teachers at a college of education in Seoul participated in this study. After the workshop of analogy in science education, they generated analogies for lessons. In order to investigate thought processes deeply, we used the think-aloud method and also conducted semi-structured interviews after their activities. Worksheets written by the pre-service teachers were collected. Their activities and interviews were recorded and videotaped. The characteristics in the processes of generating analogy were analyzed in the perspectives of student, analog, and concept. The analyses of the results revealed that they generated analogies to correct students' misconceptions and also considered misconceptions that could be caused by their analogies. They generated analogies using sources with which students are familiar. They also generated concrete and everyday analogies rather than abstract and artificial analogies. There were some cases that they did not clearly grasp the target concepts and expressed the concepts which were not covered in the unit. On the bases of the results, we suggest some educational implications for pre-service science teacher education.

Poster Presentation : **EDU.P-494**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

A case study on the university professors' teaching performance in the college of science and engineering

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In this study, we analyzed university professors' teaching performance in the college of science and engineering from the cultural historical activity theory (CHAT) perspective. Two professors volunteered to participate in this study. After collecting their syllabi, we observed their classes and conducted semi-structured interview before and after their classes. We extracted the content of six CHAT components, such as 'subjects', 'objects', 'rules', 'communities', 'division of labor', and 'tools' from all the data. And we constructed an analysis framework based on the extracted contents. The results revealed that both professors had difficulties because of the contradictions among the components of subject, object, rules, and community in the activity system. Both professors used strategies to settle the contradiction related to students' ability. However the extent of providing opportunities to students to participate was different between two professors. As they observed positive changes in students' learning, both professors preferred to continue their own strategies. In other words, the success experiences of two professors influenced their teaching performance. We discussed some suggestions to improve the quality of the class in the college of science and engineering. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(NRF-2017R1D1A3B03029531).

Poster Presentation : **EDU.P-495**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

The Characteristics of Discussions in Socioscientific Issues Classes: Focused on Group and Classroom Discussions

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¹*Department of Chemistry Education, Seoul National University, Korea*

In this study, we investigated the argumentations of group and classroom discussions in socioscientific issues (SSI) discussion classes. Twenty-seven high school students participated in the SSI discussion classes on nuclear power generation. We observed and recorded the classes and also conducted semi-structured interviews. For the analyses, we revised a previous framework that was developed to analyze dialogic argumentations in the context of SSI. The analyses of the results indicated that there were more discourse schemes in the classroom discussions than the group discussions which are related to awareness and openness to multiple perspectives, evidence based reasoning, and on-going inquiry and skepticism. And there were few discourse schemes related to moral and ethical sensitivity in the group and classroom discussions. Various grounds, data, and information were presented in the classroom discussions. Students concentrated on carrying their claims and were not able to sympathize with and accept other opinions. Therefore, there were few discourse schemes to reach consensus. In addition, they perceived classroom discussions as competitive and actively rebutted other claims or grounds. The levels of argumentation were also high in the classroom discussions. The group discussions were held in relaxed atmosphere, and they asked the opponents more for clarification or additional information and evidences. However, classroom discussions were held in serious atmosphere, and they actively queried the validity of the claims or grounds. Based on the results, some suggestions to implement SSI discussion classes were discussed.

Poster Presentation : **EDU.P-496**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

The Characteristics of Middle School Students' Graph Construction According to Daily-life and Scientific Contexts: Focused on the Views on the Nature of Scientific Measurement

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In this study, we investigated the characteristics of graph construction of middle school students on daily-life and scientific contexts by the views on the nature of scientific measurement. A test consisting of three similar data sets regarding daily-life and scientific contexts was developed, and administered to 151 ninth graders. They were expected to construct proportional, inverse-proportional, and broken line graphs for each data set. Graphs constructed were analyzed in the aspects of constructing general form, interpolating/extrapolating, selecting axes variables, scaling axes, and plotting points. Analyses of the results revealed that the students with set paradigm tended to construct curved line, while those with point paradigm constructed broken line in inverse-proportional graph questions. In this case, the students were likely to construct curved line in daily-life context and broken line in scientific context. In interpolating/extrapolating, most students with set paradigm performed both interpolation and extrapolation better than those with point paradigm in scientific context. Most students with set paradigm performed both interpolation and extrapolation regardless of contexts, while those with point paradigm performed better in daily-life context. In selecting axes variables, scaling axes, and plotting points, there were no significant differences between set and point paradigms or daily-life and scientific contexts. On the bases of the results, educational implications for improving graph construction skills of middle school students are discussed.

Poster Presentation : **EDU.P-497**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

Analysis of student recognition of their character competence based on the Collaborative Problem-Solving for Character Competence (CoProC) instruction model in chemistry class

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After developing assessment tools of student character competence enhanced by the Collaborative Problem-Solving for Character Competence (CoProC) instruction model, this research focused on student recognition of their character competences which includes openness, sympathy, tolerance, consideration, sincerity, self-control, honesty, responsibility, and cooperation, developed by our previous research. Acquired from 89 middle school students who participated the CoProC classes for 2 semesters, data including two different self-checklists were analyzed.

Poster Presentation : **EDU.P-498**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

The Effect of Collaborative Mentoring Program for Beginning Science Teachers' Professional Development

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The purpose of this study was to investigate how a collaborative mentoring program influenced beginning science teachers teaching. The one-year program consisted of five one-on-one mentoring meetings, science education seminars, mentoring group discussions, and self-evaluation activities. The participants were twelve mentor teachers and twelve mentee teachers (beginning science teachers) at the middle school. We collected data such as video recordings of mentee teachers' classes, recording of one-on-one mentoring, and mentor and mentee teacher's journals. RTOP(The Reformed Teaching Observation Protocol) was used to evaluate beginning science teachers' lessons. RTOP consists of six aspects of class, which are inquiry oriented class aspect, subject knowledge aspect, problem-solving emphasis aspect, implementing the learning community aspect, reconstitution of classroom conversation aspect, and the perspective of the teacher's clear understanding aspect. Result showed that through the collaborative mentoring program, mentee teachers have shown high levels of improvement in the inquiry oriented class aspect, problem-solving emphasis aspect and implementing the learning community aspect. In addition, there have been low levels of improvement in subject knowledge aspect, reconstitution of classroom conversation aspect, and the perspective of the teacher's clear understanding aspect.

Poster Presentation : **EDU.P-499**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

Comparison of teaching practicum in primary school between South Africa and South Korea

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South Africa is one of the countries that students have the lowest achievement in science and math. Worries and concerns have been paid over the last two decades, but remarkable changes have not been found. They are now struggling to train and equip their primary preservice teachers to teach science effectively. During the visit to one of teacher education institute in Eastern Cape, South Africa as a visiting scholar in 2018, the presenter experienced teaching practicum of primary preservice teachers. Before the practicum, he attended one course for preparing teaching practicum called “school experience” and observed class activities. During the six weeks of practicum, he visited four primary schools with a different school district and learning environment. In this presentation, details of school practicum will be shared in terms of practicum process, school selection, role of host teacher and supervisor, and class evaluation.

Poster Presentation : **EDU.P-500**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

Application of programmes based on scientific history of Volta and Daniel cells

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One of the biggest goals of science education is to foster students' scientific thinking skills. To this end, in the 2015 revision curriculum, a curriculum called 'Science Inquiry Experiment' was established, and many students in the school are doing a lot of R & E activities. Students have a lot of difficulties in inquiry, but it is difficult for teachers to teach them effectively. Reproducing scientists' inquiries directly helps to develop scientific thinking skills. Science education based on science history is a very intensive and effective way to teach inquiry methods. Although there is a subject called science history in Korea, it is not taught in real science inquiry in class. The development of the voltaic cell and the change to the Daniel cell are very important in the history of science. However, many textbooks still teach VA cells and Daniel cells in a simple way or separately. We want to develop a program that tracks the scientific thinking that scientists did while developing the Volta and Daniel cells. By applying the developed program to high school and pre-service teachers, we want to study how their scientific thinking progresses.

Poster Presentation : **EDU.P-501**

Chemistry Education

Exhibition Hall 2, THU 11:00~12:30

A Study on the Relationship between National Science Curriculum and Scientific Inquiry through Analysis of Entries in the National Science Fair as a Case of the Implementation of Scientific Education Process

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In this study, we analyzed the entries of the chemical section of the National Science Fair as an example of the implementation of science education courses to confirm the link between the planned curriculum and the curriculum of students conducted in the form of scientific inquiry. The analysis criteria set whether or not to include concepts of national curriculum of the student research, research motivation and subject, detailed academic field, and classified the work by two researchers majored in chemistry. The analysis showed that the distribution of the academic field of the elements of the curriculum was similar to that of the academic field of the entries, so it was estimated that the curriculum's content affected students' selection of research subjects. In addition, 11.9 percent of the cases derived research subjects from the content of the curriculum, and 52.7 percent of cases conducted only with concepts within the curriculum, which did not meet the criteria for the goal of the national curriculum. Therefore, two points were proposed to strengthen the link between student scientific exploration activities and planning national education courses.

Poster Presentation : **ENVR.P-502**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Photoelectrochemical CO₂ Reduction to Formaldehyde and Acetaldehyde

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Artificial photosynthesis is a most important topic in recent years. It shows the best prominent way to produce clean, efficient and renewable energy. Since last several years many photocatalytic materials have been introduced in artificial photosynthesis [1-3]. Artificial photosynthesis divides into two parts such as water oxidation and CO₂ reduction. Water oxidation is light driven reaction and CO₂ reduction is a dark reaction, so photocatalytic material can be work as a photoanode and cathode electrode can be useful for CO₂ capture, activation as well as multi electron process part. In this work, Ca/Fe doped TiO₂ as a photoanode has been prepared by simple co-precipitation method with high temperature calcination. Cathode electrodes have been prepared by various combinations of rGO(reduced graphene oxide)/PVP(poly(4-vinyl)pyridine)/Nafion on Cu foil. The major product of formaldehyde (□ 475 □ M) and acetaldehyde (□ 480 mM) were observed in case of Cu/rGO and Cu/rGO/PVP/Nafion cathode electrode respectively, with applied bias potential 0.68 V vs RHE. In this work, detail mechanism for CO₂ reduction has been studied with careful attention of CO₂ capture, activation and multi electron shuttling.

Poster Presentation : **ENVR.P-503**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

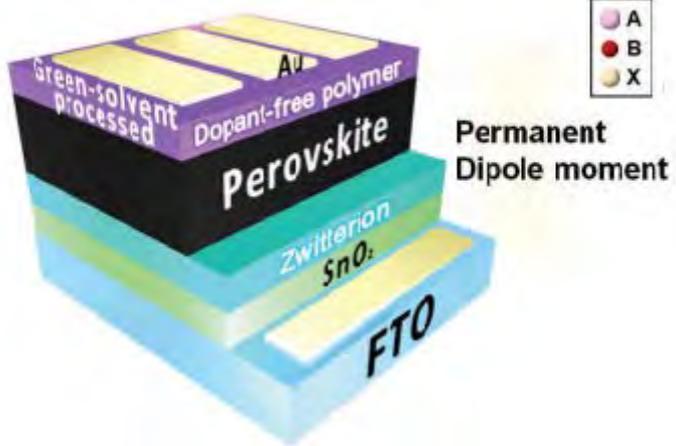
High efficient planar hybrid perovskite solar cell using zwitter ion in electron transporting layer to achieve high thermal stability

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For thermal stability in perovskite solar cells, we employed a zwitterion-modified electron transport (ETL) layer with a dopant-free hole transport layer (HTL). To modify ETL, a zwitterionic compound, 3-(1-pyridinio)-1-propanesulfonate is doped in to SnO₂ ETL. There are few advantages for a zwitterionic compound since they form interfacial dipoles. First, zwitterion causes work function of SnO₂ work function shifts. Second, they pulls electrons from perovskite layers to the border between ETL and perovskite layer to enhance ETL performance. At last, positively charged atoms in zwitterion passivate Pb-I defects enhancing device stability. Because of these advantages, we achieved power conversion efficiency of 21.43% with spiro-OMeTAD perovskite solar cell. Furthermore, we also achieved 20.5% efficiency using dopant-free HTL among the highest efficiency using dopant-free polymeric HTLs using green solvents. Therefore, this work suggests promising strategy to solve thermal stability issue in planar perovskite solar cell.



Poster Presentation : **ENVR.P-504**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Shape modeling of ZnSn(OH)₆ nanoparticles and their application as quartz crystal microbalance measurements

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In this paper, urchin-like hollow sphere shaped ZnSn(OH)₆ were synthesized by the 2-step hydrothermal method. During the synthesis process, the sphere shaped ZnSn(OH)₆ was used as a template and formed by Pearson's hard and soft acid and base (HSABs) theory. A peculiar point is that unlike the sphere shape, the urchin-like hollow sphere shape has two phases of ZnSn(OH)₆ and SnO₂. Also, SnO₂ rods were located at outside of urchin-like hollow sphere structure and confirmed by EDS mapping. In addition, it was characterized by Scanning electron microscopy (SEM), X-ray diffraction (XRD), and Raman spectrum. Finally, we measured quartz crystal microbalance (QCM) based on the advantage of unique shape. As a result, urchin-like hollow sphere shape has a much better sensing properties than the sphere shape.

Poster Presentation : **ENVR.P-505**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Iron Phosphide in Iron-Treated Heteroatoms-Doped Porous Bio-Carbon as Efficient Electrocatalyst for the Oxygen Reduction Reaction.

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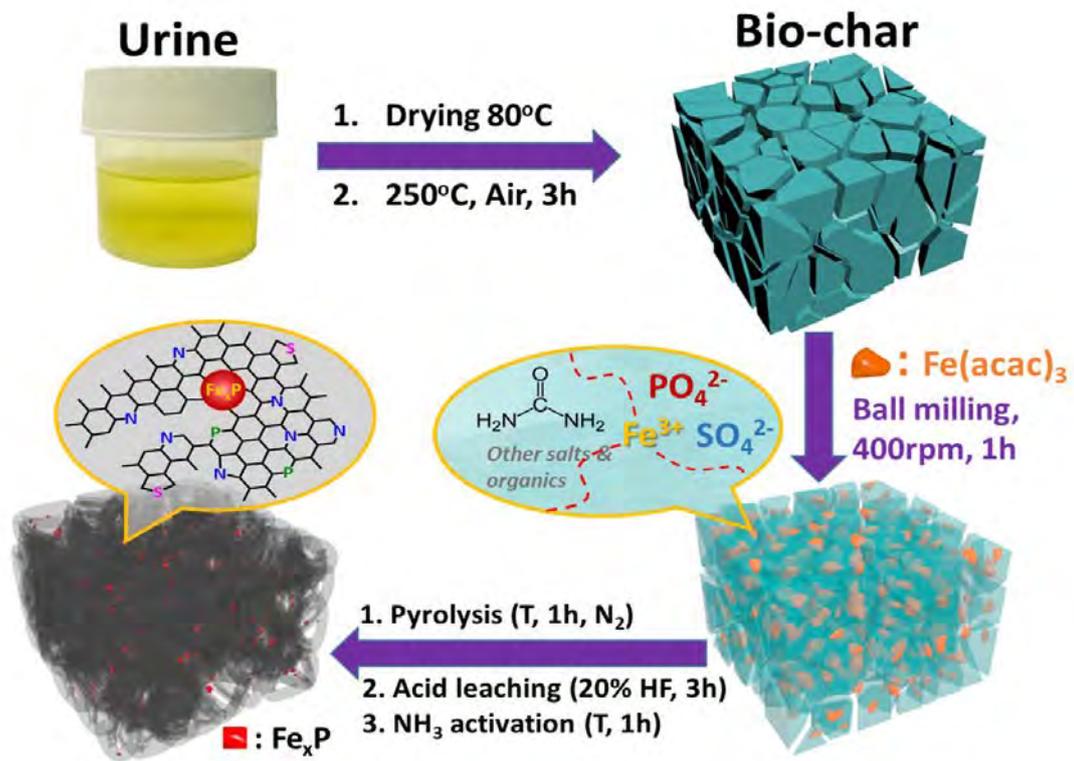
The development of electrocatalysts from inexpensive, natural sources has been an attractive subject owing to economic, environmental, sustainable, and social merits. ^[1] Herein, Fe-treated heteroatoms (N, P, and S)-doped porous carbons are synthesized for the first time by pyrolysis of bio-char derived from abundant human urine waste as a single precursor for carbon and heteroatoms, using iron(III) acetylacetonate as an external Fe precursor, followed by acid leaching and activation with a second pyrolysis step in NH₃. In particular, the sample prepared at a pyrolysis temperature of 800 °C (FeP-NSC-800) contains iron phosphide (FeP, Fe₂P)^[2] in the high-porosity heteroatoms-doped carbon framework along with Fe traces, and exhibits excellent oxygen reduction reaction (ORR) activity and stability in both alkaline and acidic electrolytes as demonstrated in half- and single-cell tests. Such excellent ORR catalytic performance is ascribed to a synergistic effect of multiple active Fe–P, Fe–N, and pyridinic and graphitic N species in the electrocatalyst as well as facile transport channels provided by its hierarchical porous structure with micro-/mesopores. In addition, the sample exhibits high long-term durability and methanol crossover resistance.

References

[1]T.-N. Tran, M.Y. Song, K.P. Singh, D.-S. Yang, J.-S. Yu, *J. Mater. Chem. A* **2016**, *4*, 8645.

[2]K.P. Singh, E.J. Bae, J.-S. Yu, *J. Am. Chem. Soc.* **2015**, *137*, 3165.

Figure 1. Schematic illustration of the preparation process for FeP-NSC-*T* electrocatalysts



Poster Presentation : **ENVR.P-506**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Predicting mercury bioavailability in artificial and natural soils for earthworm *Eisenia fetida* using the diffusive gradients in thin films

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The diffusive gradients in thin films (DGT) probe is an effective tool for evaluating metal bioavailability, however, its applicability is subject to the type of metal and organism involved. In this study, the accumulated mass of Hg in DGT probes and in the earthworm species *Eisenia fetida* was monitored in artificial soils and natural river soils together with soil properties, to test if DGT technique can be used as a predicting method for the bioavailability of Hg to earthworms. In the Hg exposure tests using artificial soils prepared with different peat moss concentrations of 5, 10, 15, and 20% and varying pH values of 4.6, 5.6, and 6.2, the DGT-soil accumulation factor (DSAF) and biota-soil accumulation factor (BSAF) both increased as the peat moss content decreased and the pH increased. Across diverse soil properties, steady-state Hg in earthworm tissue showed a strong positive correlation with the DGT-measured Hg flux, while meager correlations were found between Hg concentration in earthworms and that in pore water (and acid-extractable), indicating that DGT-measured Hg flux is a better tool than conventional methods for predicting Hg bioavailability by earthworms inhabiting diverse types of soil. To test if DGT probes can be applicable for Hg bioavailability prediction in natural soils, DGT and earthworms were deployed in eight surface soils collected from Hyeoungsan (HS) River, along with the measurements of conventional soil properties (e.g., oxidation-reduction potential, pH, labile Hg, water holding capacity and organic matter content). The results revealed that the BSAF of Hg was able to be estimated by DGT, and moreover, 71 and 64% of the Hg accumulation in DGT and earthworm, respectively, was explained by a multiple regression model applying soil properties. Overall results demonstrate that DGT-measured Hg flux, related to the soil properties as well as Hg concentration, is a practical tool for predicting Hg bioavailability for earthworms inhabiting diverse types of soils.

Poster Presentation : **ENVR.P-507**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

IDENTIFICATION OF MAJOR SOURCES OF MONOMETHYLMERCURY IN LAKES AND RIVERS OF SOUTH KOREA BY MASS BUDGETS ESTIMATION

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To identify main sources of monomethylmercury (MMHg) in lake and river water, mass budgets of MMHg were estimated for Okjeong and Boryoung Lakes, and Yeongsan and Geum Rivers using water, sediment and rainwater data collected in 2017 to 2018. The data variances of water quality parameters (e.g., pH, and concentrations of suspended particles, nitrate, sulfate and chlorophyll-a) and MMHg concentration were also analyzed by the principal component analysis (PCA), using surface water data collected from 2013 to 2018 from 16 lakes and 4 rivers. Among four main sources of MMHg (i.e., wet deposition, in-situ methylation, stream inflow and sediment diffusion), sediment diffusion was estimated as a major one for lake water and surface water inflow for river water. The PCA supports these mass balance results by showing that data variations of MMHg and pH are similar in the lake water loading plots, while the most robust positive correlation was found between MMHg and suspended particles in river water. Overall results suggest that the transport of MMHg along with allochthonous organic matter via stream discharge, and in-situ sediment methylation is a key process to increase MMHg concentration in lake and river, respectively.

Poster Presentation : **ENVR.P-508**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

High performance microbial fuel cell

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Metal complex-microbial fuel cells (MFCs) have been investigated in this work with intent manufacturing high performance MFC batteries. The performance of metal complex MFCs was evaluated by polarization and discharge experiments using a battery consisting of 3 MFC unit cells. The results indicated that the performance of the [Fe(III)(4,4'-dimethyl-2,2'-bipy)3]-MFC was much better than the other MFCs containing Cr(VI) or Fe(III) as an electron acceptor. At a discharging current of 3 mA (2 A/m²), the average discharging potential was found to be 0.927 V under a parallel-connection, sustaining more than 20 hours with an open circuit voltage of 1.210 V. Fe(III)(4,4'-dimethyl-2,2'-bipyridyl)3-MFC showed much higher electrochemical parameters than Cr(VI)-MFC and Fe(III)-MFC. Highest maximum power of 3937 mW/m² could be obtained from the battery consisting of 3 MFCs in parallel.

Poster Presentation : **ENVR.P-509**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Probing Nanomechanical Interaction at the Interface between Biological Membrane and Potentially Toxic Chemical

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Various xenobiotics interact with biological membranes, and precise evaluations of the molecular interactions between them are essential to foresee the toxicity and bioavailability of existing or newly synthesized molecules. In this study, surface forces apparatus (SFA) measurement and Langmuir trough based tensiometry are performed to reveal nanomechanical interaction mechanisms between potential toxicants and biological membranes for ex vivo toxicity evaluation. As a toxicant, polyhexamethylene guanidine (PHMG) was selected because PHMG containing humidifier disinfectant and Vodka caused lots of victims in both S. Korea and Russia, respectively, due to the lack of holistic toxicity evaluation of PHMG. Here, we measured strong attraction ($W_{ad} \sim 4.2 \text{ mJ/m}^2$) between PHMG and head group of biological membranes while no detectable adhesion force between the head group and control molecules was measured. Moreover, significant changes in π -A isotherm of 1,2-Dipalmitoyl-sn-glycero-3-phosphatidylcholine (DPPC) monolayers were measured upon PHMG adsorption. These results indicate PHMG strongly binds to hydrophilic group of lipid membranes and alters the structural and phase behavior of them. More importantly, complementary utilization of SFA and Langmuir trough techniques are found to be useful to predict the potential toxicity of a chemical by evaluating the molecular interaction with biological membranes, the primary protective barrier for living organisms.

Poster Presentation : **ENVR.P-510**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Natural organic matter effects on the removal of mercury in groundwater by pumice-supported nanoscale zero-valent iron

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Previous studies have reported the outstanding Hg removal efficiency of nanosized zero-valent iron (nZVI), related to the reductive sorption of Hg(II). However, how natural organic matter (NOM) in contaminated water changes Hg removal has not been tested despite the ubiquitous presence of NOM in wastewater. To investigate the potential effects of NOM on Hg(II) removal by nZVI, a series of batch tests was carried out using a mixture of 250 nM of Hg(II) and 3.6 g L⁻¹ of pumice-supported nZVI (p-nZVI) in the absence and the presence of 1, 10, and 100 mg L⁻¹ of Suwannee River NOM (SRNOM). The 80 minute tests showed that Hg(II) removal efficacy declines with increasing NOM concentration, and in the presence of 100 mg L⁻¹ of NOM, headspace Hg(0) and Hg removal rate decrease from 23 to 12 $\mu\text{mol m}^{-3}$ and from 89 to 36%, respectively. Similar trends were observed in the 15 day tests, attributable to surface passivation of p-nZVI by NOM. In contrast, adding 100 μM of glutathione (GSH) to the mixture of Hg(II) and p-nZVI increased Hg(II) removal efficiency from 85 to 96% on day 15, attributable to the formation of Hg(II)-GSH complex that can be removed by ferric (i.e., lepidocrocite) surface of p-nZVI. Furthermore, adding GSH to the mixture of Hg(II), p-nZVI, and SRNOM effectively removed Hg(II), demonstrating the addition of thiolic organic compounds, likely to form oxidative complexes with Hg(II) and Hg(0), can be an effective way to overcome NOM inhibition effects in the application of nZVI for Hg(II) remediation.

Poster Presentation : **ENVR.P-511**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Electrochemical and photoelectrochemical CO₂ reduction with rhenium-based organometallic complexes in aqueous media.

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Carbon capture and utilization (CCU) is one of the critical environmental and energy issue due to the greenhouse gas effect. Notably, the (photo)electrochemical reaction of CO₂ reduction in an aqueous electrolyte has got great attention as an alternative approach for the effective CCU. In photoelectrochemical or electrochemical reactions there are several advantages, 1) the selectivity of products can be adjusted by applied potential and 2) the driving force for CO₂ reduction can be obtained from a renewable energy source like solar light. However, in an aqueous electrolyte condition, hydrogen evolution reactions can compete with CO₂ reduction. Therefore, developing the selective catalysts is a key factor for efficient CO₂ reduction reactions. The rhenium based organometallics has been utilized for CO production from the CO₂ reduction, but most of the cases were carried out in organic solvent conditions. In this study, we have investigated the activity of Re-based complexes for CO₂ reduction in an aqueous electrolyte, with a carbon electrode and a semiconductor photocathode as an electron source.

Poster Presentation : **ENVR.P-512**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Fe₃O₄ nanoparticles anchored on 3D porous carbon/MoS₂ composites as anodes for lithium-ion batteries with superior cycling performance

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Molybdenum disulfide (MoS₂) has been recognized as a promising anode material for lithium-ion batteries due to its high theoretical capacity and cost-effectiveness. However, its low electric conductivity and high volume expansion lead to unsatisfied electrochemical performance. Herein, 3D porous carbon/MoS₂ composites with uniform Fe₃O₄ nanoparticles (C-MF) were prepared through a facile mix-bake-wash method. The porous carbon matrix loaded with few-layered MoS₂ improves electrical conductivity and promotes lithium ion diffusion, exhibiting a high specific capacity of 939.6 mA h g⁻¹ on average at 0.1 A g⁻¹ and a high rate capability (515.9 mA h g⁻¹ at 5 A g⁻¹). Furthermore, the Fe₃O₄ nanoparticles anchored on 3D porous carbon/MoS₂ composites enhance the specific capacity and efficiently alleviate diffusion of lithium polysulfides during long-term cycling, showing outstanding cycling stability (590.1 mA h g⁻¹ after 500 cycles at 2 A g⁻¹). It is expected that 3D porous carbon/MoS₂ composites anchored with other metal oxides can also be synthesized through this facile strategy for various other related applications.

Poster Presentation : **ENVR.P-513**

Environmental Energy

Exhibition Hall 2, THU 11:00~12:30

Ultrafast Microwave-assisted Carbonization and Reduction for Carbon-encapsulated Silicon-graphene nanocomposites as Lithium-ion Battery Anode

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Conventional thermal treatment for carbonization and reduction of graphene oxide is not energy and time efficient. This work presents ultrafast (~ 4 s) simultaneous carbonization of carbon precursor and reduction of graphene via microwave irradiation using a cheap commercial microwave oven. Polydopamine-coated silicon nanoparticles are mixed with electrochemically exfoliated graphene and fabricated into a freestanding anode film through simple vacuum filtration. Many preserved sp² domains of electrochemically exfoliated graphene enable efficient microwave absorption which produces heat to carbonize Polydopamine in few seconds. The produced heat also reduces oxidized electrochemically exfoliated graphene to recover more sp² domain, which increases electrical conductivity. As a consequence, the as-prepared carbon-encapsulated silicon-graphene lithium-ion battery anode film delivers a reversible specific capacity of 1744 mAh g⁻¹ at a current density of 0.1 A g⁻¹ and good cycling stability of 662 mAh g⁻¹ at 1.0 A g⁻¹ after 200 cycles. This extremely fast method can be a better alternative to conventional tedious thermal treatment for graphene-related nanocomposite synthesis.