

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PLEN-1**

Area: Plenary Lecture

Type: Plenary Lecture, Time: THU 16:00, Chair: Jongseung Kim

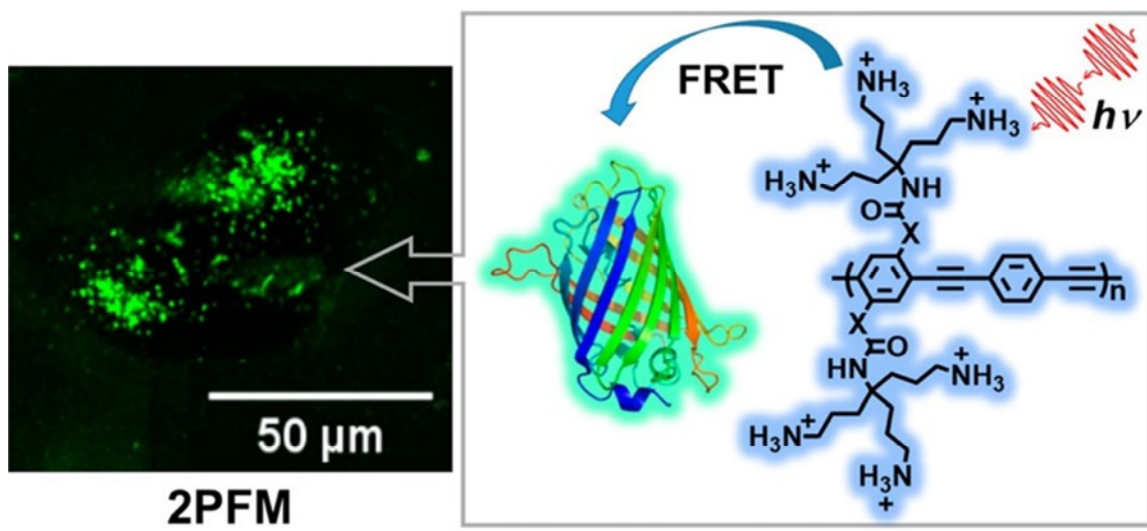
Conjugated Polyelectrolytes in Biosensing and Disinfection

Kirk S. Schanze

Department of Chemistry, University of Texas at San Antonio, United States

Conjugated polyelectrolytes (CPEs) featuring poly(phenylene ethynylene) and poly(thiophene) backbones substituted with ionic solubilizing groups are water soluble. These materials display a variety of interesting properties, including self-assembly into nanoscale aggregates, ability to process into layer-by-layer films and optical/stimuli responsive behaviour in the presence of ions, surfactants and biomacromolecules. We have explored the use of cationic CPEs as fluorescent sensors for polyphosphates (pyrophosphate, ATP and ADP). In addition, cationic CPEs exhibit strong light-activated biocidal activity vs. a broad spectrum of bioagents, including bacteria, virus particles and spores. The talk will overview recent work in this area, including the interaction with cationic CPEs with mammalian cells.

- [1] Jiang, H.; Taranekar, P.; Reynolds, J. R.; Schanze, K. S. "Conjugated Polyelectrolytes: Synthesis, Photophysics, and Applications", *Angew. Chem.* 2009, 48, 4300-4316, DOI: 10.1002/anie.200805456.
- [2] Wu, D.; Schanze, K. S. "Protein Induced Aggregation of Conjugated Polyelectrolytes Probed with Fluorescence Correlation Spectroscopy: Application to Protein Identification", *ACS Appl. Mater. Interfaces* 2014, 6, 7643-7651, DOI: 10.1021/am5009437.
- [3] Parthasarathy, A.; Pappas, E. H.; Hill, E. H.; Huang, Y.; Whitten, D. G.; Schanze, K. S. "Conjugated Polyelectrolytes with Imidazolium Solubilizing Groups. Properties and Application to Photodynamic Inactivation of Bacteria", *ACS Appl. Mater. Interfaces* 2015, 7, 28027-28034, DOI: 10.1021/acsami.5b02771.
- [4] Wang, S.; Li, Z.; Liu, X.; Phan, S.; Lv, F.; Belfield, K. D.; Wang, S.; Schanze, K. S. "Two-Photon Absorption of Cationic Conjugated Polyelectrolytes: Effects of Aggregation and Application to 2-Photon-Sensitized Fluorescence from Green Fluorescent Protein", *Chem. Mater.* 2017, 29, 3295-3303, DOI: 10.1021/acs.chemmater.7b00676.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: AWARD-1

Area: Award Lecture

Type: Award Lecture, Time: FRI 11:00, Chair: Wonyoung Choe

Recent Advances of Metallosupramolecules of Macrocycles: Networking, Post-Synthetic Modifications, Bioinspiration, and Adaptive Responses

Shim Sung Lee

Department of Chemistry, Gyeongsang National University, Korea

Nature has been a source of scientific inspiration because the relations between structure and function are associated with their behaviors in molecular level. Inspired by the nature's elaborated fashion, we report several synthetic receptors involving crown ethers, calixarenes, pillararenes, and acyclic chelates which recognize specific organic guests via the metal-driven adaptation.¹⁻⁶

The regioisomers of bis-dithiamacrocyclic *o*-bis-L (W-shape binding site) and *m*-bis-L (U-shape binding site) react with CuI to yield 1-D polymers, in which each isomer is linked by cubane [Cu₄I₄] cluster and square [Cu₂I₂] cluster, respectively (Fig. 1).² The results illustrate the possibility for the adaptive formations of the clusters through the binding site design or alternation.

Post-synthetic modifications (PSMs) via an SCSC transformation provide a powerful tool, not only for creating of new materials, but also for understanding mechanistic pathways. We report an anion exchange process accompanying cation reduction and dimerization via the SCSC transformation.³

Calix[6]-crown-5 allowed us to isolate *molecular capsules* incorporating both homo- and heteromultinuclear alkali metal ions in a head-to-head fashion in which the bowl-type host units act as a glue to stabilize the elegant capsule arrangement (Fig. 2).⁶ To the best of our knowledge, these are the first capsule-like species which involve several homo- or hetero-metal ions.

The combination of the dicopper platform (**1**) and 1,4-bis(4-pyridyl)piperazine (bpp) afforded the first example of a 1-D polyrotaxane whose string and bead are constructed from the same components (Fig. 3).⁴ The formation of the polyrotaxane is driven by π - π stacking between the *string* and the *beads* with electronic and steric complementarity evident between these components.

Among the photochemical methods, [2+2] cycloaddition has been employed to generate cyclobutane based coordination polymers from the metal complexes. Our advancements in the construction of

polymeric chains of cyclobutane rings via photo-dimerisation reaction containing metal complexes, coordination polymers and MOF are also introduced (Fig. 4).⁵

In biological molecular recognition, induced fit via adaptive structural changes of the receptor is more acceptable than lock-&-key principle. We report a metal-driven cascade complex with a flexible macrocycle whose organic guest recognition is anion dependent (Fig. 5).⁶ In solution, its dimercury(II) perchlorato complex recognizes dabco, but its iodo complex shows no reactivity. Crystal structures reveal that the dabco recognition is associated with a swing door manner of each coordinated anion.

Pillar[5]-bis-dithiacrown (**L**) shows non-selective complexations with a series of α,ω -dicyanoalkanes [CN(CH₂)_nCN, n = 2-6, shortly **C2-C6**] (Fig. 6).⁶ Upon disilver(I) complexation, **L** shows an adaptation to form a *cascade complex* with **C2** in which two Ag(I) ions bound to the thiacycrown rings with ~10 Å separation are linked by one **C2**, exhibiting a shape-changing of the host.

References

1. Park, S.; Lee, S. Y.; Park, K.-M.; Lee, S. S. *Acc. Chem. Res.* 2012, 45, 391.
2. Kim, S.; Siewe, A. D.; Lee, E.; Ju, H.; Park, I.-H.; Park, K.-M.; Ikeda, M.; Habata, Y.; Lee, S. S. *Inorg. Chem.* 2016, 55, 2018.
3. Lee, H.-H.; Park, I.-H.; Kim, S.; Lee, E.; Ju, H.; Jung, J. H.; Ikeda, M.; Habata, Y.; Lee, S. S. *Chem. Sci.* 2017, 8, 2592.
4. Ju, H.; Clegg, J. K.; Park, K.-M.; Lindoy, L. F.; Lee, S. S. *J. Am. Chem. Soc.* 2015, 137, 9535.
5. Park, I.-H.; Chanthapally, A.; Zhang, Z.; Lee, S. S.; Zaworotko, M. J.; Vittal, J. J. *Angew. Chem. Int. Ed.* 2014, 53, 414.
6. Unpublished data.

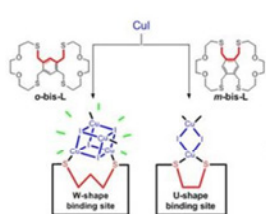


Fig. 1.
Inductive cluster formation.

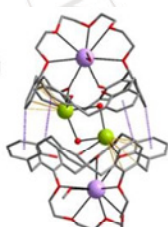


Fig. 2.
Molecular capsule.

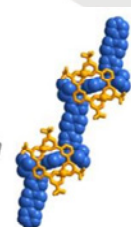


Fig. 3.
Polyrotaxane.



Fig. 4.
Photopolymerization.

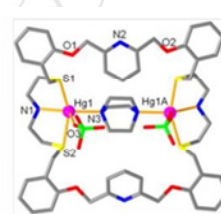


Fig. 5.
Induced fit model.

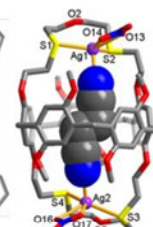


Fig. 6.
Cascade complex.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY1-1**

Area: Human-friendly Polymers and Their Applications

Type: Award Lecture in Division, Time: THU 09:00, Chair: Byeong-Su Kim

Exploration of Novel Ionic Polymers and Their Structure-Property Relationship

Minjae Lee

Department of Chemistry, Kunsan National University, Korea

Exploration of Novel Ionic Polymers and Their Structure-Property Relationship Minjae Lee | Department of Chemistry, Kunsan National University

Abstract: Various types of polymerizable ionic liquid monomers and their polymers are synthesized for the potential applications in electrolyte components of electroactive devices. To perform both traditional chain-growth radical polymerizations and step-growth polycondensations, proper monomer functionalities are introduced to the ionic liquid monomers. For the polymerized ionic materials, structure-property relationships for both pendant and main-chain polycations with various counter-anions are carefully investigated by various spectroscopic and thermal analyses. Ionic polymers with pendant imidazolium units show different morphologies and thermal properties through the different pendant structures; some structural characteristics are important to the property changes. Main-chain polycations with various anions show remarkable morphology and electrical property changes; a lamellar microphase-separation gives a big increase in ionic conductivity. Copolyesters of imidazolium-ionic and PEG blocks show interesting thermal behaviors and ionic conductivity changes by varying a chemical structure. The potential applications of the synthesized polymers are expanding to energy storage and harvesting devices, such as full-solid electrolytes for supercapacitors, dye-sensitized solar cells and organic/inorganic hybrid solar cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY1-2**

Area: Human-friendly Polymers and Their Applications

Type: Symposium, Time: THU 09:40, Chair: Byeong-Su Kim

Electrochemical surface modification of bioelectrodes using hyaluronic acid derivatives to improve electrode functions and tissue compatibility

Jae Young Lee

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

Bioelectrodes have been widely used to effectively mediate electrical signals with biological systems for various biomedical applications such as biosensors and prosthetic probes. However, the electrical properties of bioelectrodes are frequently degraded in the biological milieu due to non-specific adsorption of proteins and cell growth on the bioelectrode surfaces. Hence, the development of simple and effective strategies for bioelectrode surface modification becomes important to leverage biocompatibility. To this end, electrochemical electrode surface modification using hyaluronic acid (HA) derivatives (i.e., pyrrole-HA (PY-HA) and dopamine-HA) that are electrochemically active were performed. The modified electrodes exhibit highly hydrophilic surfaces. In addition, the electrochemical impedance of the modified electrodes remains similar to those of bare electrodes. The PY-HA-coated electrodes minimized adhesion and migration of fibroblasts and astrocytes for a minimum of up to 3 months. Also, PYHA-modified wire electrodes were implanted into rat motor cortices for three weeks and were found to markedly reduce the expression of glial fibrillary acidic protein compared to uncoated electrodes. The DA-HA-modified electrodes prevent non-specific protein adsorption and minimize adhesion of fibroblasts. Our novel electrochemical passivation of electrodes using electroactive HA derivatives will contribute to the further development of antifouling and biocompatible bioelectrodes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY1-3**

Area: Human-friendly Polymers and Their Applications

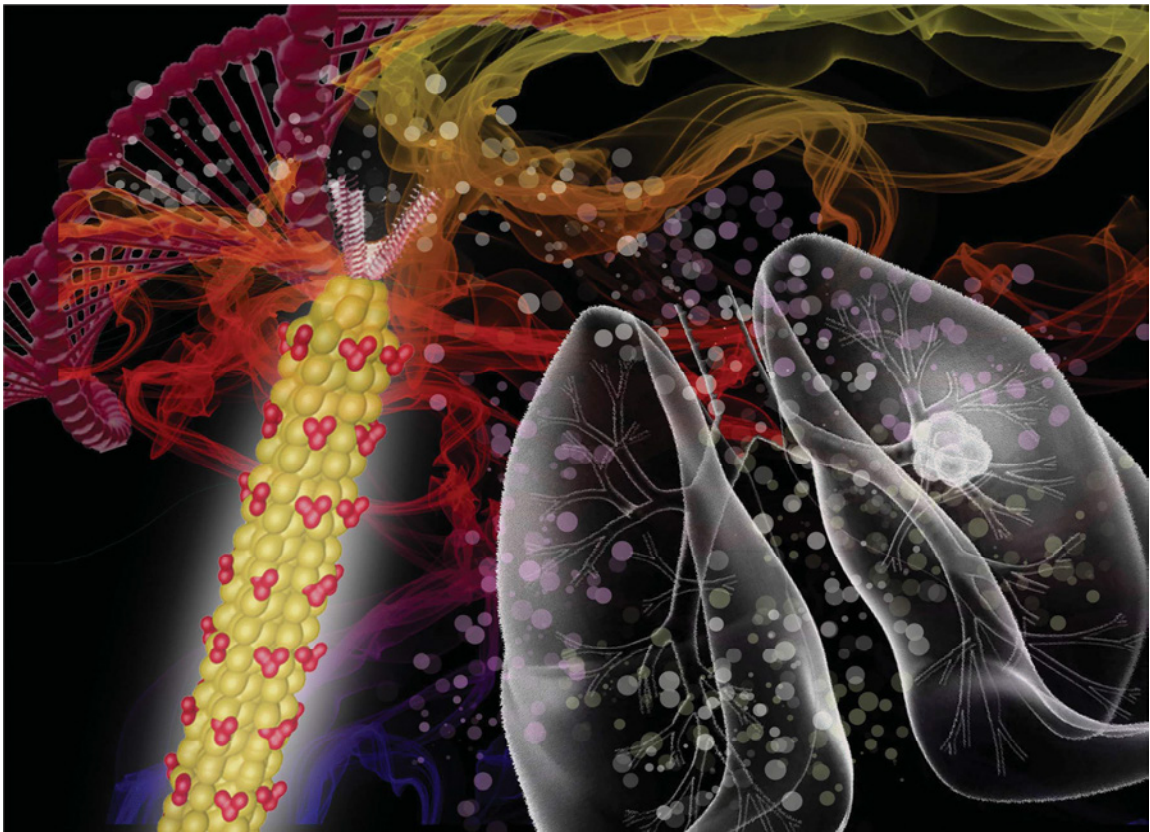
Type: Symposium, Time: THU 10:00, Chair: Byeong-Su Kim

Virus based Novel Colorimetric Sensor for Cancer cell detection

Jin-Woo Oh

Department of Nanoenergy Engineering, Pusan National University, Korea

Color sensor like pregnancy test kit or litmus paper for pH test relies on color change depending on various chemical and physical conditions. Recently, we developed the novel colorimetric sensor which is functionalized with M-13 bacteriophage-based structure color [1], and it could detect TNT down to 300 p.p.b. over similarly structure chemicals [2]. Cancer cells release abnormal gas composition compared with that of normal cells. Therefore, cancer can be diagnosed by breath testing for a unique composition of volatile gas produced by each species of cells. Here, we developed the novel cancer recognition sensor using virus-based structural color matrix. Due to its liquid crystalline behavior and surface modification ability, M-13 bacteriophage based color sensor exhibited remarkable selectivity and sensitivity to target samples including chemicals which compose VOCs of NCI. Upon exposure of small amounts of target molecules, the resulting colored matrices exhibited distinct different color changes that can be applied to effectively discriminate the target. Although the cancer cell sensing system was used as proof-of-concept in this study, this approach can be generalized to the detection of many harmful and biological toxicants.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY1-4**

Area: Human-friendly Polymers and Their Applications

Type: Symposium, Time: THU 10:20, Chair: Jin-Woo Oh

Hydrogel micropatterns incorporating electrospun fibers for biomedical applications

Won-Gun Koh

Chemical & Biomolecular Engineering, Yonsei University, Korea

In this study, we describe a simple method for fabricating multiscale scaffolds that are capable of controlling the spatial positioning of mammalian cells and proteins or peptides. Photopatterning of poly(ethylene glycol)(PEG) hydrogel on the electrospun nanofibers produced micropatterned nanofiber matrices made of hydrogel microwells filled with a nanofibrous region, which is capable of generating cell and protein micropatterns due to the different interactions that cells and proteins have with PEG hydrogels and nanofibers. Different types of biomolecules could be immobilized onto resultant micropatterned nanofiber scaffold, carrying out cell patterning, metabolite detection, and growth factor delivery.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY1-5**

Area: Human-friendly Polymers and Their Applications

Type: Symposium, Time: THU 10:40, Chair: Jin-Woo Oh

Reinvent of silk protein as an optical and electrical material

Sunghwan Kim

Department of Physics, Ajou University, Korea

The interplay between the electrical and photonic phenomena endogenous to biological matter and the ones externally induced or transduced through technological interfaces has driven developments in understanding natural systems driving new approaches in biosensing and imaging techniques. Silk fibroin, the natural protein extracted from the *Bombyx mori* caterpillar, has been shown to be an attractive material for applications in bio electronics and photonics due to its biocompatibility and unique mechanical and optical characteristics. The favorable characteristics of silk fibroin films afford the adaptation of micro- and nano-fabrication techniques commonly used in organic electronics and photonics manufacturing. Here, state of the art and opportunities offered by silk proteins as a promising biomaterial will be focused.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY2-1**

Area: Special Symposium by Leading Mid-career Polymer Scientists

Type: Symposium, Time: THU 13:30, Chair: Bumjoon Kim

Stable Bulk Heterojunction Prepared by Sequential Deposition Process

Kyungkon Kim

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

A morphologically stable bulk heterojunction (BHJ) with a large heterojunction area is prepared by reducing the portion of the small band gap polymer (PTB7) and fullerene intermixture through a sequential deposition (SqD) of the nanostructured PTB7 and the fullerene layer. The nanostructured PTB7 layer is prepared using a ternary solvent composed of chlorobenzene, 1,8-diiodooctane (DIO) and 1-chloronaphthalene (1-CN). Adding DIO and 1-CN enhances the ordering of PTB7 chains and results in a nanostructured polymer surface. The grazing incidence X-ray diffraction results reveal that the SqD of the nanostructured PTB7 and fullerene layers forms the BHJ with little intermixing between the polymer and the fullerene domains compared to the BHJ formed by the deposition of the blended PTB7 and fullerene solution (BSD). The OPV utilizing the SqD processed BHJ (SqD-OPV) exhibits a power conversion efficiency (PCE) of 7.43%, which is similar to that when the BSD processed BHJ (BSD-OPV) is utilized. Furthermore, the SqD-OPV exhibits an excellent thermal stability. The SqD-OPV maintains its initial PCE even after thermal annealing at 140 °C for 10 days, whereas the BSD-OPV maintains 78% of its initial efficiency under the same condition.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY2-2**

Area: Special Symposium by Leading Mid-career Polymer Scientists

Type: Symposium, Time: THU 13:55, Chair: Bumjoon Kim

A novel strategy in design of polymeric hole transporting materials for green processable, dopant-free perovskite solar cells

Taiho Park

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

Spiro-OMeTAD as hole transporting material (HTM) has been widely employed up to PCE = 22.1 %, but it is only processed in chlorinated or harmful solvents such as chlorobenzene (CB), dichlorobenzene (DCB), or toluene, despite of its low molecular weight relative to polymeric HTMs. Therefore, it is necessary to replace it to green solvent processable HTM. Here, we report a green solvent processable, polymeric HTM consisting of benzodithiazole and benzo[1,2-b:4,5:b']dithiophene. We design a novel D (e-donor) – A (e-acceptor) type conducting polymer to obtain its proper highest occupied energy level (HOMO) easily and to achieve its high hole mobility as we demonstrated, allowing effective hole extraction from perovskites to HTM and then hole transportation through HTM without Li-TFSI and t-BP, respectively. The resulting novel polymeric HTM is not only soluble in the various halogenated or harmful solvents but also highly soluble in a green solvent. In this talk, I will present a design strategy for a green solvent processable HTM and why it exhibits a highly stable device with a highest PCE in the absence of the dopants.[References]1) YS Kwon, J Lim, H-J Yun, Y-H Kim, T Park, Energy Environ. Sci. 2014, 7, 1454.2) G-W Kim, J Kim, G-Y Lee, G Kang, J Lee, T Park, Adv. Energy Mater. 2015, 5, 1500471.3) G-W Kim, DV Shinde, T Park, RSC Advances 2015, 5, 99356.4) G-W Kim, G Kang, J Kim, G-Y Lee, H Kim, L Pyeon, J Lee, T Park, Energy Environ. Sci. 2016, 9, 2326.5) G-W Kim, G Kang, MM Byranvand, G-Y Lee, T Park, ACS Appl. Mater. & Inter. 2017, 9, 27720.6) G-W Kim, J Lee, G Kang, T Kim, T Park, Adv. Energy Mater. 2017, accepted.7) J Lee, MM Byranvand, G Kang, SY Son, S Song, G-W Kim, T Park, J. Am. Chem. Soc. 2017, accepted.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY2-3**

Area: Special Symposium by Leading Mid-career Polymer Scientists

Type: Symposium, Time: THU 14:20, Chair: Bumjoon Kim

Cellulose paper energy storage electrodes using layer-by-layer assembly

Jinhan Cho

Dept of Chemical & Biological Engineering, Korea University, Korea

The effective implantation of conductive and charge storage materials into flexible frames has been strongly demanded for the development of flexible supercapacitors. Here, we introduce metallic cellulose paper-based supercapacitor electrodes with excellent energy storage performance by minimizing the contact resistance between neighboring metal and/or metal oxide nanoparticles using a novel assembly approach, called ligand-mediated layer-by-layer assembly. This approach can convert the insulating paper to highly porous metallic paper with large surface areas that can function as current collectors and nanoparticle reservoirs for supercapacitor electrodes. Moreover, we demonstrate that the alternating structure design of the metal and pseudocapacitive nanoparticles on the metallic papers can remarkably increase the areal capacitance and rate capability with a notable decrease in the internal resistance. The maximum power and energy density of the metallic paper-based supercapacitors are estimated to be $15.1 \text{ mW}\cdot\text{cm}^{-2}$ and $267.3 \text{ }\mu\text{W}\cdot\text{h}\cdot\text{cm}^{-2}$, respectively, substantially outperforming the performance of conventional paper or textile-type supercapacitors.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY2-4**

Area: Special Symposium by Leading Mid-career Polymer Scientists

Type: Symposium, Time: THU 15:05, Chair: Kyungkon Kim

P- and N-type Organic Photovoltaic Materials for OPV Devices

Han Young Woo

Department of Chemistry, Korea University, Korea

Over the past few decades, polymer solar cells (PSCs) have made a significant progress, showing their potential in low-cost, flexible, lightweight, portable and large-area energy-harvesting devices. Considerable efforts have been dedicated toward the design of new materials, device architectures and processing techniques in order to improve the power conversion efficiency (PCE). To further improve the PCE value, first and foremost, the molecular structures of p- and n-type photovoltaic materials should be carefully designed by considering its close relationship with the photovoltaic parameters, including short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}) and fill factor (FF). Here, we present a series of crystalline photovoltaic conjugated molecules which were designed by considering the backbone planarity, noncovalent intra- and interchain interactions (via H-bonding and dipole-dipole interactions, etc) and solution processibility, leading to highly ordered film morphologies and PCEs approaching ~10%. The molecular design and resulting morphological, electrical and device properties will be discussed in detail.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY2-5**

Area: Special Symposium by Leading Mid-career Polymer Scientists

Type: Symposium, Time: THU 15:30, Chair: Kyungkon Kim

Impact of Side Chain Engineering and Molecular Weight Control of Polymers in Performance of All-Polymer Solar Cells

Bumjoon Kim

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

All-polymer solar cells (all-PSCs) often suffer from low short-circuit current density and fill factor, which is mainly associated with inefficient exciton dissociation at the donor/acceptor interface and electron transport in the device. This feature results from anisotropic structure in both polymer donor and polymer acceptor, which is different from spherical shaped fullerenes. In this talk, we will address our recent work in developing the correlation between the polymer microstructure, BHJ morphology and the photovoltaic properties of high performance all-PSCs. As model systems of modulating the molecular weight and the alkyl side chain of polymers, the polymer microstructure and the BHJ blend morphology of all-PSCs are systematically controlled, and thereby we produced high-performance all-PSCs system with over 7% efficiency. More importantly, our all-PSCs exhibited dramatically enhanced strength and flexibility compared with polymer/PCBM devices, with 60x and 470x improvements in elongation at break and toughness, respectively. The superior mechanical properties of all-PSCs afford greater tolerance to severe deformations than conventional polymer-fullerene solar cells, making them much better candidates for applications in flexible and portable devices.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY3-1**

Area: Special Symposium for Polymer Research at the Korean National Laboratories

Type: Symposium, Time: FRI 09:00, Chair: Heesuk Kim

Polymerization of Sustainable Bioplastics from Heterocyclic Bio-based Monomers

Jeyoung Park

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

Petrochemical plastics have showed very important roles in the chemical industry over the past decades and can be found everywhere because of their low cost, durability, lightweight, and so on. Production and consumption of plastics which are essential in everyday life from disposable products to high-tech devices have been dramatically increase. As a result, various environmental global issues inevitably appeared by massive use of synthetic polymers produced from fossil resources. Biodegradable polymers, i.e., PBS, is still skeptical about the replacement of industrial products due to the limited physical properties. As an alternative, many researchers have been interested in synthetic biopolymer with good mechanical properties. Herein, we introduced and investigated some examples of high performance sustainable bioplastics polymerized from heterocyclic monomers derived from biomass resources, i.e., isosorbide and dimethyl furan-2,5-dicarboxylate, to verify their potentials for various plastic industries.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY3-2**

Area: Special Symposium for Polymer Research at the Korean National Laboratories

Type: Symposium, Time: FRI 09:25, Chair: Heesuk Kim

Self-healing Properties of Supramolecular Polymers based on Charge Transfer Complex (CTC) Interaction

Sung Woo Hong

Intelligent Sustainable Materials R&D Group, Korea Institute of Industrial Technology, Korea

A new self-healable polymeric material based on supramolecular chemistry is synthesized and its self-healing properties are examined in terms of charge transfer complex (CTC) interaction. The self-healable polymeric material used in this study is prepared from polyimides, where CTC is formed through electronically-complementary interaction between dianhydride and diamine groups in polyimide chains. The self-healing behaviors are attributed to the strong supramolecular networks resulting from the intramolecular and intermolecular CTC interactions of polyimide chains. The self-healable material based on polyimides shows excellent self-healing capabilities and fast self-healing kinetics, which explains its feasibility to be widely used for self-healing applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY3-3**

Area: Special Symposium for Polymer Research at the Korean National Laboratories

Type: Symposium, Time: FRI 10:00, Chair: Jeyoung Park

Development of High Performance Organic Solar Cells by Utilizing e-Donating Random Copolymers

Hae Jung Son

Korea Institute of Science and Technology, Korea

In order for organic solar cells to fully mature from research and development into cost effective products, a continuous improvement in solar cell efficiency must be achieved. A fundamental comprehension of design principles of new polymer materials are necessary to push this area forward. We synthesized a series of conjugated random copolymers with a backbone of 5,6-difluoro-2,1,3-benzothiadiazole moieties and studied the effect of the polymer structure on photovoltaic properties. We demonstrated that modification of the polymer backbone affected the energy levels and the morphology of polymer/fullerene blend films, resulting in power conversion efficiencies (PCEs) of 7~10%. Moreover, such high solar cell performances are effectively realized in a large area and so resulting devices achieves PCEs over 9%. This work shows the effect of fine-tuning of the chemical structure on solar cell performance.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY3-4**

Area: Special Symposium for Polymer Research at the Korean National Laboratories

Type: Symposium, Time: FRI 10:25, Chair: Jeyoung Park

Poly(N-isopropylacrylamide) copolymers for sequential and reversible foldings in ionic liquids

Soonjong So, Ryan Hayward^{1,*}

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

¹*Department of Polymer Science and Engineering, University of Massachusetts Amherst, United States*

Sequential self-transformations of 2D sheets into 3D structures are of great interest in the area of origami-inspired materials to make more complex configurations that cannot be accessed by simultaneous foldings. We demonstrate sequential and reversible bending of a microactuator by tuning the upper critical solution temperature (UCST) of poly(N-isopropylacrylamide) (PNIPAM) copolymers in the ionic liquid (IL), 1-ethyl-3-methylimidazolium bis(trifluoro-methylsulfonyl) imide. The copolymers have different hydrogen-bonding capabilities by incorporating acrylic acid and methyl acrylate, and show the higher and lower UCSTs than PNIPAM in the IL, respectively. Relying on the tunable transition temperature through copolymerization, we demonstrate a UV-patterned thermal-actuator, which has potential for origami and soft robots.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: IOMT-1

Area: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] Molecules and Materials for Safe and Sustainable Future

Type: Symposium, Time: THU 13:30, Chair: Kwangyeol Lee

METAL-OXYGEN INTERMEDIATES IN DIOXYGEN ACTIVATION CHEMISTRY

Wonwoo Nam

Department of Chemistry, Ewha Womans University, Korea

Dioxygen is essential in life processes, and enzymes activate dioxygen to carry out a variety of biological reactions. One primary goal in biomimetic research is to elucidate structures of reactive intermediates and mechanistic details of dioxygen activation and oxygenation reactions occurring at the active sites of enzymes, by utilizing synthetic metal-oxygen complexes. A growing class of metal-oxygen complexes, such as metal-superoxo, -peroxo, -hydroperoxo, and -oxo species, have been isolated, characterized spectroscopically, and investigated in various oxygenation reactions. During the past decade, we have been studying the chemical and physical properties of various reactive intermediates in oxygenation reactions, such as high-valent iron(IV)- and manganese(V)-oxo complexes of heme and non-heme ligands in oxo-transfer and C-H activation reactions, non-heme metal-peroxo complexes in nucleophilic reactions, and non-heme metal-superoxo complexes in electrophilic reactions. The effects of supporting and axial ligands on structural and spectroscopic properties and reactivities of metal-oxygen adducts have been extensively investigated as well. In this presentation, I will present our recent results on the synthesis and structural and spectroscopic characterization of mononuclear non-heme metal-dioxygen intermediates as well as their reactivities in electrophilic and nucleophilic oxidation reactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IOMT-2**

Area: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] Molecules and Materials for Safe and Sustainable Future

Type: Symposium, Time: THU 14:00, Chair: Kwangyeol Lee

Organic-Inorganic Halide Perovskite Solar Cell: Disruptive Photovoltaics

Nam-Gyu Park

School of Chemical Engineering, Sungkyunkwan University, Korea

Since the first report on the solid-state perovskite solar cell with power conversion efficiency (PCE) of 9.7% in 2012 by our group, its certified PCE now reaches 22%. It is believed that perovskite solar cell is promising next-generation photovoltaics (PVs) due to superb performance and low cost. In this talk, the history of perovskite photovoltaics will be briefly presented along with scientific progress of perovskite solar cells. Methodologies to achieve hysteresis-free, stable and high PCE perovskite solar cells will be introduced. Lewis acid-base adduct approach has been found to be very reliable and reproducible method to get high quality perovskite layer minimizing non-radiative recombination. Non-stoichiometric precursor in adduct process demonstrated grain boundary healing effect, which further improved voltage and fill factor due to long carrier life time of perovskite and improved charge transporting at grain boundary as well. Grain boundary healing process yields PCE as high as 20.4%. Moisture was effectively protected and hysteresis was significantly reduced by introducing 2-dimensional perovskite at grain boundary of 3-dimensional perovskite. Thermal stability of perovskite material was found to be stable up to 120 oC in the absence of moisture, but that of full device was sensitive to selective contacts, indicating that thermally stable selective contacts are equally important. Universal method to remove hysteresis will be also given in this talk. Beyond PV, recent progress in resistive memory, light emitting diode and photodetector based on halide perovskite will be also covered in this talk.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IOMT-3**

Area: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] Molecules and Materials for Safe and Sustainable Future

Type: Symposium, Time: THU 14:30, Chair: Kwangyeol Lee

Designed Chemical Synthesis and Assembly of Uniform-sized Nanoparticles for Medical Applications

Taeghwan Hyeon

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

Over the last 18 years, our laboratory has focused on the designed chemical synthesis, assembly and applications of uniform-sized nanocrystals. In particular, we developed a novel generalized procedure called as the “heat-up process” for the direct synthesis of uniform-sized nanocrystals of many metals, oxides, and chalcogenides. For the last 10 years, our group has been focused on medical applications of various uniform-sized nanoparticles. Using 3 nm-sized iron oxide nanoparticles, new non-toxic MRI contrast agent was realized for high resolution MRI of blood vessels down to 0.2 mm. For the last 10 years, our group has been focused on medical applications of various uniform-sized nanoparticles. Using 3 nm-sized iron oxide nanoparticles, new non-toxic MRI contrast agent was realized for high resolution MRI of blood vessels down to 0.2 mm. Very recently, we report on the biocompatibility evaluation and MR imaging of extremely small and uniform-sized iron oxide nanoparticles in large animal models including most clinically-relevant non-human primates. These biocompatible iron oxide nanoparticles are successfully used as T1 MR contrast agent for high-resolution MR angiography of macaque monkeys. We demonstrated that intravenously administered ceria nanoparticles could substantially reduce the damage from ischemic strokes, and that triphenylphosphonium-conjugated ceria nanoparticles can localize to mitochondria and suppress neuronal death in 5XFAD transgenic Alzheimer’s disease mouse model. I will present recent advances on the fabrication of ultraflexible and stretchable electronic and optoelectronic devices integrated with various functional nanomaterials and their applications to wearable and implantable healthcare devices. We reported graphene-hybrid electrochemical devices integrated with thermo-responsive micro-needles for the sweat-based diabetes monitoring and feedback therapy. We reported the designed fabrication of multifunctional wearable electronic devices for sensing, data storage, and drug-based feedback therapy of motion-related neurological disorders such as Parkinson’s disease.

We introduced electromechanical cardioplasty using an epicardial mesh made of electrically conductive and mechanically elastic silver nanowire-rubber composite material to resemble the innate cardiac tissue and confer cardiac conduction system function.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: IOMT-4

Area: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] Molecules and Materials for Safe and Sustainable Future

Type: Symposium, Time: THU 15:00, Chair: Sang Hoon Joo

Large-Area Growth of High Quality Hexagonal Boron Nitride Chemical Vapor Deposition and Its Applications

Hyeon Suk Shin

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

Large-scale growth of high-quality hexagonal boron nitride (h-BN) has been a challenge in two-dimensional (2D)-material-based electronics. In this presentation, I demonstrate wafer-scale and wrinkle-free epitaxial growth of multi-layer h-BN on a sapphire substrate by using high-temperature and low-pressure chemical vapor deposition.[1] Microscopic and spectroscopic investigations and theoretical calculations reveal that synthesized h-BN has a single rotational orientation with Bernal stacking order. A facile method for transferring h-BN onto other target substrates were developed, which provides the opportunity for using h-BN as a substrate in practical electronic circuits. A graphene field effect transistor fabricated on our h-BN sheets shows highly improved carrier mobility, because the ultra-flatness of the h-BN surface can reduce the substrate-induced degradation of the carrier mobility of 2D materials. Afterwards, I show some potential applications of h-BN for a shell layer capping Au nanoparticles in surface-enhance Raman scattering [2], an encapsulation (or passivation) layer to protect unstable transition metal dichalcogenides (TMDs) [3], and a proton exchange membrane to replace the Nafion film in a polymer electrolyte membrane (PEM) fuel cell.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IOMT-5**

Area: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] Molecules and Materials for Safe and Sustainable Future

Type: Symposium, Time: THU 15:25, Chair: Sang Hoon Joo

Nanoparticles with structurally-dictated 3-D arrangement of multiple material phases: precursors to ideally performing nanocatalysts in electrolytic water splitting and fuel cell applications

Kwangyeol Lee

Department of Chemistry, Korea University, Korea

Nanoparticle-based catalysis is intrinsically surface-confined, and thus the surface area of nanocatalyst should be maximized, which in turn raises the question of nanocatalyst structural stability during harsh catalytic condition. 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. On the other hand, nanoparticle surface energy plays a crucial role in determining catalytic activity and stability, and is affected by the surface composition, crystal facet, surface strain, defects, and etc. 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 H₂ fuel cells, which have gained a great attention due to ever increasing environmental problems associated with fossil fuel usages. Specifically we focus on the synthesis of multiphasic nanoparticles, which exhibit region-specifically located multiple material phases within a very small nanoparticle domain and are able to evolve into nanocatalysts with high surface area, high structural robustness, and fine-tuned surface energy.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INORI-1**

Area: Recent Trends in Bio-Inorganic Chemistry

Type: Symposium, Time: FRI 09:00, Chair: Seungwoo HONG

Charge transfer as key principles of C-H bond activation and cross coupling

Kiyoung Park

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

Metalloenzymes and metallocofactors in nature often demonstrate uniquely high efficiency that cannot be observed elsewhere. One example is C-H bond activation by non-heme iron enzymes; mononuclear or binuclear iron sites utilize O₂ to form high-valent intermediates that can abstract H atom from strong bonds such as the C-H bond of methane. The principle of these reactions has been elucidated on the basis of intermediate structures established by nuclear resonance vibrational spectroscopy, revealing that spin-polarized charge transfer from oxo ligand to Fe center determines intrinsic barrier for the reaction. A series of high-valent organometallic complexes that show different rates of reductive elimination process have been spectroscopically and computationally studied. A good correlation amongst the energy level of redox-active metal d orbitals, the type of supporting ligands, and cross coupling reaction rate demonstrate that the activity and selectivity of C-C bond cross coupling reaction can be understood in parallel with enzyme's strategy to raise the reduction potential of a metal center by dissociating or exchanging ligands.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR1-2**

Area: Recent Trends in Bio-Inorganic Chemistry

Type: Symposium, Time: FRI 09:25, Chair: Seungwoo HONG

Metal coordination region of concanavalin A for interaction with human norovirus

Seung Jae Lee

Department of Chemistry, Chonbuk National University, Korea

Rapid methods for the detection and clinical treatment of human norovirus (HuNoV) are needed to control foodborne disease outbreaks, but reliable techniques that are fast and sensitive enough to detect small amounts of HuNoV in food and aquatic environments are not yet available. We explore the interaction between HuNoV and concanavalin A (Con A), which could facilitate the development of a sensitive detection tool for HuNoV. Biophysical studies including hydrogen/deuterium exchange (HDX) mass spectrometry and surface plasmon resonance (SPR) revealed that when the metal coordinated region of Con A, which spans Asp16 to His24, is converted to nine alanine residues (mCon A^{MCR}), the affinity for HuNoV (GII.4) diminishes, demonstrating that this Ca²⁺ and Mn²⁺ coordinated region is responsible for the observed virus-protein interaction. The mutated carbohydrate binding region of Con A (mCon A^{CBR}) does not affect binding affinity, indicating that MCR is a major region of interaction. The results further contribute for the development of a HuNoV concentration tool, Con A-immobilized polyacrylate beads (Con A-PAB), for rapid detection of genotypes of genogroup I and II (GI and GII). This method offers many advantages over currently available methods, including a short concentration time. Norovirus can be detected in just 15 minutes with 90% recovery through Con A-PAB application. In addition, this method can be used over a wide range of pH values (pH 3.0–10.0). Overall, this rapid and sensitive detection of human norovirus will aid in the prevention of virus transmission pathways and the method developed here may have broad applicability for other foodborne viral infections.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR1-3**

Area: Recent Trends in Bio-Inorganic Chemistry

Type: Symposium, Time: FRI 09:50, Chair: Seungwoo HONG

Multiple Interconnected Pathological Factors (Metals, Amyloid- β , and Reactive Oxygen Species) in Alzheimer's Disease

Mi Hee Lim

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

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid- β ($A\beta$) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the $A\beta$ plaque and likely contribute to $A\beta$ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of $A\beta$ plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.¹⁻⁵ To find a cure for AD, we require a better understanding of the relationship between the various causative factors of this devastating disease. Towards this goal, we need suitable chemical tools capable of targeting and regulating its multiple underlying factors simultaneously.²⁻⁴ Herein, our rational design and preparation of our chemical tools will be discussed with our investigations of their interactions and reactivities with targets in vitro as well as their efficacy in vivo.⁶⁻¹⁰

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: INORI-4

Area: Recent Trends in Bio-Inorganic Chemistry

Type: Symposium, Time: FRI 10:15, Chair: Seungwoo HONG

Distinct Reactivity of a Mononuclear Peroxocobalt(III) Species towards Activation of Nitriles

Jaheung Cho

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

The activation of nitriles is a field of synthetic interest for the preparation of materials important in fine chemical synthesis and pharmaceutical production, but typical methods have the disadvantage that strong bases or acids and high temperatures must be required. In this presentation, a mononuclear side-on peroxocobalt(III) complex with a tetradentate macrocyclic ligand, [Co(III)(TBDAP)(O₂)]⁺ (1), shows a novel and facile mode of dioxygenase-like reactivity with nitriles (R-C≡N; R = Me, Et, and Ph) to produce the corresponding mononuclear hydroximatocobalt(III) complexes, [Co(III)(TBDAP)(R-C(=NO)O)]⁺, in which the nitrile moiety is oxidized by two oxygen atoms of the peroxo group. The overall reaction proceeds in one-pot under ambient conditions (ca. 1 hour, 40 °C). ¹⁸O-labeling experiments confirm that both oxygen atoms are derived from the peroxo ligand. The structures of all products, hydroximatocobalt(III) complexes, were confirmed by X-ray crystallography and various spectroscopic techniques. Kinetic studies including the Hammett analysis and isotope labeling experiments suggest that the mechanistic mode of 1 for activation of nitriles occurs via a concerted mechanism. This novel reaction would be significantly valuable for expanding the chemistry for nitrile activation and utilization.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR1-5**

Area: Recent Trends in Bio-Inorganic Chemistry

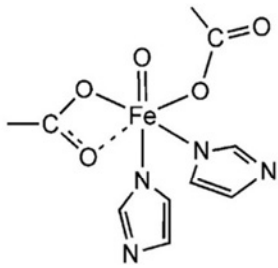
Type: Symposium, Time: FRI 10:40, Chair: Seungwoo HONG

Spin-dependent Mechanism and the Formation of Fe^{III}-oxyl radical in C-H Bond Activation by Non-heme Fe^{IV}O Complexes

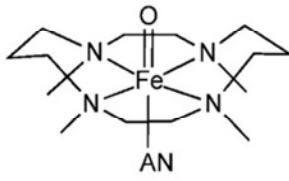
YONGHO KIM

Department of Applied Chemistry, Kyung Hee University, Korea

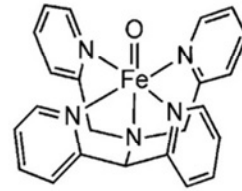
High valent Fe^{IV}O species has been proposed to play a key role in the catalytic cycle of non-heme mono-iron enzymes. Extensive studies have been performed to reveal the catalytic mechanism of the enzyme and to reproduce its catalytic reactivity using biomimetic Fe^{IV}O complexes with synthetic ligands. In this study, the mechanism of C-H activation has been investigated at an atomic detail for four synthetic complexes with an Oh symmetry and two with a Tbp symmetry including a TauD-J model (see below), based on the DFT potential energy surfaces of both S =1 and S =2 spin states. This study demonstrated that all the high spin Fe^{IV}O complexes, irrespective of their symmetry (Tbp or Oh), utilize a species like an Fe^{III}-oxyl radical for C-H activation, which is formed en route to the TS before the actual HAT occurs. However, no such species is formed in the intermediate spin state (S = 1). The reason why the reactivity of high spin complexes depends on ligand symmetry even with nearly identical mechanism will be discussed.



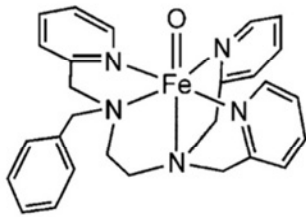
$[(\text{TauD-J})\text{Fe}^{\text{IV}}\text{O}]$



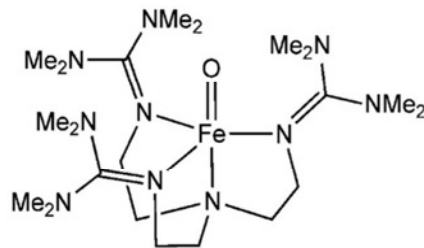
$[(\text{TMC})(\text{AN})\text{Fe}^{\text{IV}}\text{O}]^{2+}$ (1)



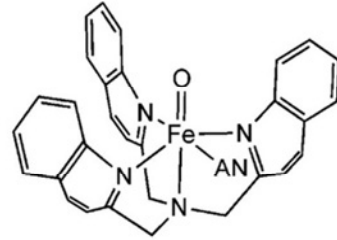
$[(\text{N4Py})\text{Fe}^{\text{IV}}\text{O}]^{2+}$ (2)



$[(\text{Bn-TPEN})\text{Fe}^{\text{IV}}\text{O}]^{2+}$ (3)



$[(\text{TMG}_3\text{tren})\text{Fe}^{\text{IV}}\text{O}]^{2+}$ (4)



$[(\text{TQA})(\text{AN})\text{Fe}^{\text{IV}}\text{O}]^{2+}$ (5)



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR2-1**

Area: Recent Trends in Organometallic Chemistry

Type: Award Lecture in Division, Time: FRI 14:30, Chair: Myung Hwan Park

Photonic Applications of Organoboron and Boron Cluster Compounds

Min Hyung Lee

Department of Chemistry and EHSRC, University of Ulsan, Korea

Tri-coordinate organoboron compounds have received great attention in the fields of optoelectronic applications, such as anion sensors and OLEDs, due to their high Lewis acidity and intriguing photophysical properties. During recent years, our group has developed novel triarylboron-based anion sensors that can feature enhanced binding affinity or turn-on luminescence response. As well, triarylboron compounds were also utilized as electron-acceptors or emitters for high-efficiency OLEDs. On the other hands, the boron cluster compound, such as *o*-carborane, has attracted as a new class of steric and electronic auxiliary in the luminescent materials. Our group first reported that the *o*-carborane containing cyclometalated Ir(III) complexes can be used as highly efficient, color-tunable phosphorescent emitters in OLEDs. It was revealed that *o*-carborane can affect both the inductive and conjugative electronic effects. In particular, the quantum efficiency of Ir(III) complexes was shown to be strongly affected by the carborane groups. In this presentation, recent development and photonic applications of organoboron and boron cluster compounds will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR2-2**

Area: Recent Trends in Organometallic Chemistry

Type: Award Lecture in Division, Time: FRI 14:55, Chair: Myung Hwan Park

Flexible Metal-Organic Frameworks

Hoi Ri Moon

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

Coordination chemistry, which is the science concerned with the interactions of organic ligands with metal centers, is classical but still very attractive approach to construct novel functional materials. Rational and creative design of organic and metal building blocks successfully affords a variety of coordination polymers or metal-organic frameworks (MOFs) that have practical usefulness as well as scientific significance. Recently, flexible MOFs have attracted great attention because they show distinctive properties that cannot be achieved with rigid MOFs and other porous inorganic materials. In this talk, we will present synthetic strategies for flexible MOFs and their interesting properties. Especially, responsive MOFs upon external stimuli such as light irradiation, gas adsorption/desorption and specific organic molecules sensing will be introduced.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR2-3**

Area: Recent Trends in Organometallic Chemistry

Type: Symposium, Time: FRI 15:20, Chair: Min Hyung Lee

Cobalt-Catalyzed C–F Bond Borylation of Aryl Fluorides

Eunsung Lee

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

Fluorine atoms can be found in a variety of organic molecules such as pharmaceuticals, agrochemicals, and polymeric materials. In line with an importance of fluorinated compounds, there have been significant advances on C–F bond formation for the past decades. However, unlike a development of C–F bond formation reactions, C–F bond functionalization has been limited to either highly activated C–F bonds or C–C bond formation. In 2015, C–F functionalization of unactivated fluoroarenes has been developed by the Marting group and the Niwa and Hosoya group demonstrating Ni-catalyzed defluoroborylation of fluoroarenes and its application to F-18 radiochemistry and further organic transformations. Although the methods are efficient and top-notch, there are still some limitations: high reaction temperatures, limited functionality-tolerance, and operational difficulty. In order to overcome the barriers, we have been explored Co-based catalysis and here we present cobalt-catalyzed unactivated aryl C–F bond borylation. This reaction can be set up under the air condition and do not require a presynthesized organometallic complex. A mild and practical Co-catalyzed borylation of various fluoroarenes enables a new reaction strategy in synthetic chemistry.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR2-4**

Area: Recent Trends in Organometallic Chemistry

Type: Symposium, Time: FRI 15:40, Chair: Min Hyung Lee

Photosensitization Effects of Ir(III) Complexes in Selective Reduction of CO₂ by Re(I)-Complex-Anchored TiO₂ Hybrid Catalyst

Ho-Jin Son

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

A series of cationic Ir(III) complexes ($[\text{Ir}(\text{btp})_2(\text{bpy-X}_2)]^+$ (Ir-X⁺: btp = (2-pyridyl)benzo[b]thiophen-3-yl; bpy-X₂ = 4,4'-X₂-2,2'-bipyridine (X = OMe, tBu, Me, H, and CN)) were applied as visible-light photosensitizer in solution to the selective CO₂ reduction to CO in the presence of an electron donor (BIH) and a hybrid catalyst (TiO₂/ReP) prepared by anchoring of Re(4,4'-Y₂-bpy)(CO)₃Cl (Y = CH₂PO(OH)₂) on TiO₂ particles. Irradiation of the system in N,N-dimethylformamide (DMF) at >400 nm resulted in the successful reduction of CO₂ to CO with efficiencies in the order X = tBu ~ Me > OMe > H; Ir-CN⁺ has no photosensitization effect. An interesting observation is that Ir-tBu⁺ and Ir-Me⁺ are less efficient than Ir-OMe⁺ at an early stage of the reaction but reveal persistent photosensitization behavior for a longer period of time unlike the latter. Comparable experiments showed that (1) the Ir-X⁺ sensitizers are commonly superior compared to Ru(bpy)₃²⁺, a widely used transition-metal photosensitizer and (2) the system comprising Ir-tBu⁺ and TiO₂/ReP is much more efficient than a homogeneous-solution system using Ir-tBu⁺ and Re(4,4'-Y'₂-bpy)(CO)₃Cl (Y' = CH₂PO(OEt)₂). Implications of the present observations and reaction mechanisms are discussed in detail.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR2-5**

Area: Recent Trends in Organometallic Chemistry

Type: Symposium, Time: FRI 16:00, Chair: Min Hyung Lee

Luminescent Salen-Based Aluminum and Indium Complexes: Control of Optical Properties by Manipulation of Functional Groups

Myung Hwan Park

Department of Chemistry Education, Chungbuk National University, Korea

Various organometallic complexes based on group 13 metals, such as Al and Ga, have been widely reported as prominent optoelectronic materials due to their excellent electronic and photophysical properties. The luminescent properties of these luminophores can be controlled by a systematic modulation of the ligand frameworks. The incorporation of various substituents into the ligand as a scaffold for transition-metal complexes can induce fascinating photophysical properties, such as emission color tuning and quantum efficiency modifications, leading to an expansion of their use as promising luminescent materials. In a continuous effort to explore a novel class of color-tunable luminophores, we investigated salen-based aluminum and indium complexes with various functional groups. In particular, to the best of our knowledge, there have been no reported studies on monomeric indium complexes that display multicolor emission features due to the simple alteration of their substituents. In this presentation, the details of the foregoing chemistry will be presented along with their intriguing optical properties.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS1-1**

Area: Recent Progress in Electronic Structure Theory

Type: Award Lecture in Division, Time: THU 13:30, Chair: Young Min Rhee

Radical-based peptide mass spectrometry and IRMPD spectroscopy

Han Bin Oh

Department of Chemistry, Sogang University, Korea

Last fifteen years, I have established the biological mass spectrometry laboratory at Sogang University. The main focuses of my research have lied in the development of radical-based peptide mass spectrometry and the IRMPD spectroscopy. In the beginning of my independent career, I have studied how electron capture dissociation mass spectrometry (ECD-MS) worked for the gaseous peptide system and some interesting peptide model systems such as PAMAM dendrimers. Later, we developed a new radical-peptide tandem mass spectrometry method called "free-radical initiated peptides sequencing mass spectrometry (FRIPS MS)". We have demonstrated that FRIPS MS can be a very successful tandem mass spectrometry for peptide sequencing, elucidation for post-translational modifications, and top-down mass spectrometry. Towards the goal of establishing FRIPS MS as a practical proteomics tool, we have modified the structures of the FRIPS reagent, enabling a single step peptide sequencing even in positive ion mode. The detailed result will be shown in the symposium. In addition, the structures of gaseous peptide species were probed using IRMPD spectroscopy. Recently, chiral differentiation of L-/ D- amino acids by complexation with a cyclodextrin was demonstrated using IRMPD spectroscopy. Very lately, our laboratory have incorporated artificial intelligence computations and microfluidics technologies into the MS system, which expanded the scope of the mass spectrometry system.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS1-2**

Area: Recent Progress in Electronic Structure Theory

Type: Symposium, Time: THU 14:10, Chair: Young Min Rhee

Understanding Nonadiabatic Processes by Quantum Mechanical Nonadiabatic Dynamics

Cheol Ho Choi

Department of Chemistry, Kyungpook National University, Korea

Observing chemical reactions in real time is one of the ultimate goals of physical chemistry. Experimentally, a great deal of time-resolved spectroscopies as well as ultrafast X-ray have been developed to observe the events. The interests on such chemical reaction dynamics grow rapidly, since they are also strongly related with the light energy conversion mechanisms of photovoltaics and artificial photosynthesis. In general, they belong to “nonadiabatic processes” with the timescale of ~100 fs. Contrasting to the experimental efforts, easily accessible theoretical tools for them are rare. In this talk, we describe an efficient and practical method for “nonadiabatic processes” by combining MD, QM/MM, NACT(Nonadiabatic Coupling Term) and SP-TDDFT. In addition, we also present its applications on photochemical reactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS1-3**

Area: Recent Progress in Electronic Structure Theory

Type: Symposium, Time: THU 14:30, Chair: Young Min Rhee

Electronic structures of TiO₂ nanoparticles by DFT approaches

JIN YONG LEE

Department of Chemistry, Sungkyunkwan University, Korea

DFT approaches have been successfully applied for many research areas in chemistry. Recently developed various functionals could give more reliable results in many different subjects, however, it is still lack of fundamental unified functional. For example, band gaps of TiO₂ bulk or nanoparticles are critical for the photocatalytic activities in water splitting. For bulk TiO₂, LDA and GGA functionals underestimated band gaps, and resulted incorrect description of mid gap states of oxygen vacancies in reduced oxides. On the other hand, hybrid functionals, B3LYP (20% of HF) and PBE0 (PBE+25% of HF) overestimated the band gaps, and HSE (PBE0 + screening parameter) predicted oxygen vacancy defect state levels too deep in the gap. The most accurate many body approaches (GW) may overcome this band gap problem, but computationally too expensive. We optimized the HF percentage in PBE functional to obtain accurate band gap of bulk TiO₂. Then, using this functional we studied the electronic structure of the ground and excited states of TiO₂ nanoparticles. We will discuss on the minimum size of cluster to keep the facet in clusters and exciton binding energy of nanoparticles.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS1-4**

Area: Recent Progress in Electronic Structure Theory

Type: Symposium, Time: THU 14:50, Chair: Yousung Jung

Development of DFT functional applicable to large molecular and periodic systems

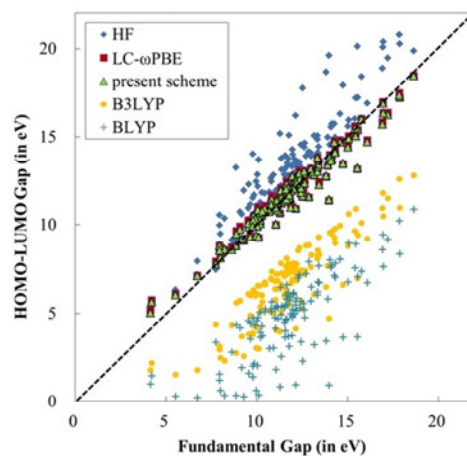
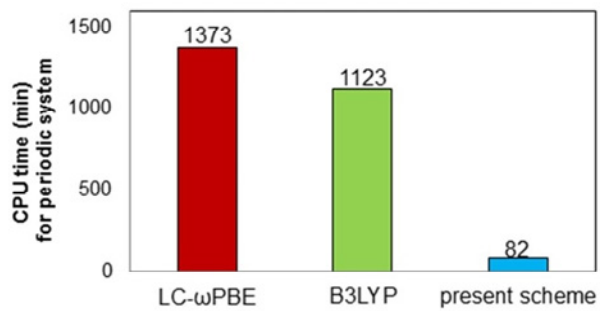
Jong-Won Song

Chemistry Education, Daegu University, Korea

Nowadays, density functional theory (DFT) is a strong theoretical tool applicable to researches on biomolecule and material sciences. In particular, hybrid DFT functionals initiated active chemical applications of DFT, in that it can reproduce energy and property of finite systems within chemical accuracy as well as with low computational cost compared with wave function theory. However, in spite of its high applicability, DFT has shown severe inappropriateness of producing some following basic properties: inter- and intra-molecular van der Waals interaction, inter- and intra-molecular charge transfer excitation energy and its oscillator strength, (hyper-)polarizability, isomerization energy of organic molecules, core-excitation energy, HOMO-LUMO gaps of molecules, and so on. As a result of our efforts to solve these problems, we proposed a new hybrid functional named long-range corrected (LC) DFT and showed successful improvement on the problems mentioned above.[1] It is well known that still high demanding of time cost to evaluate long-range HF exchange is a big obstacle for LC-DFT to be applied to large molecular systems and solid state materials. Unlike acceleration methods for Coulomb integration, such as fast multipole method, developing acceleration methods for the HF exchange is still a pioneering area. We will show our recent progress against this problem, specially on developing a new linear-scaling method of HF exchange integration for LC-DFT hybrid functional.[2] Additionally, we will present the recent results of linear-scaled LC-DFT on adsorption energy between CO molecule and Cu surface.[1] J.-W. Song, T. Hirose, T. Tsuneda, and K. Hirao, *J. Chem. Phys.* 126, 154105 (2007). [2] J.-W. Song and K. Hirao, *J. Chem. Phys.* 143, 144112 (2015).

$$\text{LC-}\omega\text{PBE} : O_{12}^{\text{HF}} = \frac{\text{erf}(\mu r_{12})}{r_{12}}$$

$$\text{present scheme} : O_{12}^{\text{HF}} = \beta_1 \exp(-\alpha_1 r_{12}) + \beta_2 \exp(-\alpha_2 r_{12})$$



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS1-5**

Area: Recent Progress in Electronic Structure Theory

Type: Symposium, Time: THU 15:10, Chair: Yousung Jung

A local exact exchange potential method for accurate excited state calculations

WOO YOUN KIM

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

Density functional theory (DFT) has been an essential tool for electronic structure calculations in various fields. In particular, its hybrid method including the Hartree–Fock (HF) exchange term remarkably enhanced the reliability of DFT for chemical applications and computational material design. However, accuracy for excited state calculations is yet to be improved. A trial with another new density functional may not be desired, as is evident from previous attempts. Instead, we tried to find a way to improve the accuracy of existing functionals. There are two different types of exchange–correlation potentials that can be derived from hybrid functionals. In conventional approaches, the HF exchange operator is adopted as a part of Kohn–Sham (KS) potential. On the other hand, the optimized effective potential (OEP) method provides another way to incorporate the exact exchange in a mean field picture by constructing a local potential from the non-local HF exchange energy. Thus, one may construct a local version of HF that is equivalent to the exchange-only OEP KS-DFT. It has been known that the exchange-only OEP KS theory gives similar occupied orbitals to HF, while its virtual orbitals are different from those of HF. Since KS virtual orbitals are closer to optical excitations, we expect that the OEP exact exchange would be more suitable to describing excited states than that of HF. Here, we show that such a local multiplicative potential can be derived from existing hybrid functionals using the OEP method. We investigate its performance for molecular excited states. Furthermore, we find that the new approach enormously accelerates computational speed of grid-based methods compared to the conventional one, which is desirable for large-scale calculations.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYSI-6**

Area: Recent Progress in Electronic Structure Theory

Type: Symposium, Time: THU 15:30, Chair: Yousung Jung

Recent progress in nonadiabatic molecular dynamics with multiple nuclear trajectories

Seung Kyu Min

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

Theoretical understanding of excited state phenomena is of paramount importance in investigating photochemical/physical phenomena such as photosynthesis, vision processes, and charge transfer in solar cells. So far various theoretical/computational methods for the excited state molecular dynamics have been developed, and one of the most promising tool for practical calculation is a trajectory-based mixed quantum-classical approach due to its simplicity and practicality. Among them, Ehrenfest dynamics and fewest switch surface hopping approach are by far the most successful algorithm in this field. In this presentation, we provide alternative trajectory-based approaches to investigate molecular dynamics involving multiple excited states based on the exact factorization of a full molecular wave function[1]. This exact factorization scheme allows us to *derive* the electron-nuclear coupling term which plays a crucial role in nonadiabatic behavior in excited state molecular dynamics. As a result, our approaches can describe a nice nuclear wave packet splitting as well as electronic decoherence[2,3,4] in various non-adiabatic situations. In addition, we discuss a recent progress in excited state molecular dynamics toward large molecular systems or extended systems.

[1] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett., 105, 123002 (2010)

[2] S. K. Min*, F. Agostini, E. K. U. Gross, Phys. Rev. Lett., 115, 073001 (2015)

[3] F. Agostini, S. K. Min*, A. Abedi, E. K. U. Gross, J. Chem. Theory Comput., 12, 2127 (2016)

[4] S. K. Min, F. Agostini, I. Tavernelli, E. K. U. Gross, J. Phys. Chem. Lett., 8, 3048 (2017)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS2-1**

Area: Physical Chemistry of Bioimaging and Biospectroscopy

Type: Symposium, Time: FRI 09:00, Chair: Nam Ki Lee

RNA Stem Structure Governs Coupling of Dicing and Gene Silencing in RNA interference

Hye Ran Koh^{*}, Amirhossein Ghanbariniaki¹, Sua Myong^{1,*}

Department of Chemistry, Chung-Ang University, Korea

¹*Department of Biophysics, Johns Hopkins University, United States*

Pre-micro(mi)RNAs possess secondary structures consisting of a loop and a stem with multiple mismatches. Despite the well characterized RNA interference (RNAi) pathway, it still remains unclear how the structural features of pre-miRNA contribute to dicing and subsequent gene silencing efficiency. Using single molecule fluorescence in situ hybridization, we demonstrate that cytoplasmic mRNA, but not nuclear mRNA, is reduced during RNAi. Dicing rate and silencing efficiency both increase as a function of the loop length in a correlated manner. In contrast, mismatches in the stem drastically diminish the silencing efficiency without impacting the dicing rate. We show that such decoupling effect is not due to the loading to RNA induced silencing complex, RNA uptake or cellular dicing. We postulate that the stem mismatches perturb the hand-over of the cleaved miRNAs from Dicer to Argonaute which leads to poor strand selection. Our results imply that the stem structures prevalent in cellular miRNAs are intended for suboptimal silencing efficiency.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS2-2**

Area: Physical Chemistry of Bioimaging and Biospectroscopy

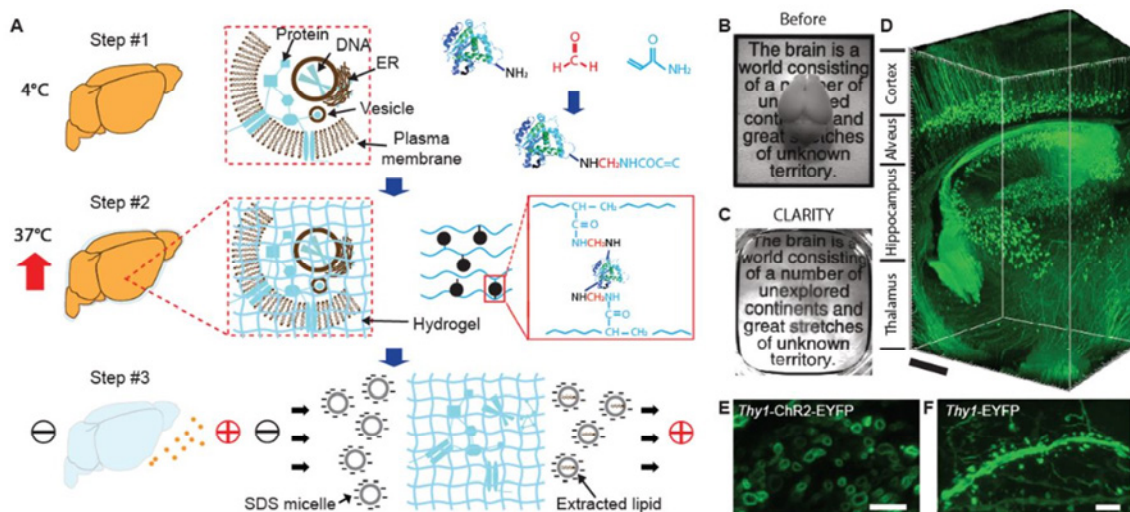
Type: Symposium, Time: FRI 09:20, Chair: Nam Ki Lee

Tissue clearing, labeling and expansion techniques for the extraction of 3D biological information

Sung-Yon Kim

Department of Chemistry, Seoul National University, Korea

Clearing, labeling and expansion techniques for large-scale biological tissues enable simultaneous extraction of molecular and structural information without disassembly of the sample, facilitating the integration of molecular, cellular and systems biology across different scales. Recent years have witnessed an explosive increase in the number of new such methods and their applications, reflecting heightened interest in organ-wide clearing and labeling across many fields of biology and medicine. I will provide an overview and comparisons of existing clearing, labeling and expansion techniques with the emphasis on CLARITY, stochastic electrotransport and SWITCH, introduce new techniques that we are developing and discuss challenges and opportunities for the investigations of intact biological systems.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS2-3**

Area: Physical Chemistry of Bioimaging and Biospectroscopy

Type: Symposium, Time: FRI 09:40, Chair: Nam Ki Lee

Super-resolution Fluorescence Microscopy For Visualizing Long-term Cellular Dynamics

Sang-Hee Shim

Department of Chemistry, Korea University, Korea

Super-resolution fluorescence microscopy opens new windows for visualizing ultrastructural dynamics. When applied to living cells, super-resolution fluorescence microscopy suffers from the limited length of time-lapse series due to high intensities of illumination and photobleaching of fluorophores. Here, we use a fluorogen-binding protein, UnaG for overcoming the photobleaching limit by controlling the switching kinetics and by supplying a large excess of fluorogenes. UnaG fluorescence can be switched off by blue light and then, recovered by replacing the damaged fluorogen with a fresh one in solution for hundreds of cycles. These switching properties enabled long-term super-resolution imaging based on single-molecule localization, with significant improvement (about 10-fold) in the number of independent super-resolution snapshots. By targeting UnaG via genetic incorporation, we demonstrated super-resolution imaging of various organelles (e.g. endoplasmic reticulum, mitochondria, peroxisome, etc) and structural proteins (e.g. vimentin, keratin, lamin, clathrin, etc). These capabilities enable us to observe cellular dynamics that progress in the time scale of minutes to hours.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS2-4**

Area: Physical Chemistry of Bioimaging and Biospectroscopy

Type: Symposium, Time: FRI 10:05, Chair: Nam Ki Lee

Monitoring state transitions in plants using *in vivo* spectromicroscopy

Tae Kyu Ahn

Department of Energy Science, Sungkyunkwan University, Korea

In chloroplasts of plants and algae, state transition is an important regulatory mechanism to maintain the excitation balance between PSI and PSII in the thylakoid membrane. Light-harvesting complex II (LHCII) plays a key role as the regulated energy distributor between PSI and PSII. It is widely accepted that LHCII, which is bound to PSII localized mainly in the granal thylakoid, migrates to bind with PSI localized mainly in the stroma-exposed thylakoid under preferential excitation of PSII. The phenomena have been extensively characterized by many methods. However, the exchange of LHCII between PSII and PSI has not been directly observed *in vivo* at physiological temperatures. Herein we applied fluorescence spectromicroscopy to *Arabidopsis* mesophyll protoplasts in order to observe *in vivo* changes in fluorescence spectra of granal and stromal thylakoid regions during the state transition. The microscopic fluorescence spectra obtained from a few sections with different depths were decomposed into PSI and PSII spectra and self-absorption effects were removed. We were able to determine amplitude changes of PSI and PSII in fluorescence spectra solely due to state transition. Subdomain analysis of granal and stromal thylakoid regions clarified variant behaviors in the different regions. I. E. Kim, T.K. Ahn, S. Kumazaki, *Plant & Cell Physiology* 2015, 56(4), 749-768

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS2-5**

Area: Physical Chemistry of Bioimaging and Biospectroscopy

Type: Symposium, Time: FRI 10:30, Chair: Nam Ki Lee

Reversibly control of enzyme activity by pH-responsive DNA nanocages

So Yeon Kim

Institute of Biomedical Engineering Research, Korea Institute of Science and Technology, Korea

To control enzyme activity regardless of the enzyme characteristics, cage-like DNA nanostructures have been used by encapsulating and releasing enzyme from the structure. However, these methods are irreversible, and thus have limitation in comparison with the reversible regulation observed in nature. Here, we present a method to covalently attach an enzyme inside of the DNA nanocage, whose structure can be reversibly switched by pH changes. We demonstrate that the enzyme accessibility to the surrounding environment, binding affinity to the corresponding antibody and even the enzyme activity can be reversibly controlled via pH dependent opening and closing of the DNA nanocage. Due to the size and pH response flexibility of DNA, our can be used as a broad-impact platform for controlling enzyme functions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS3-1**

Area: Recent Trend in Surface and Interface Physical Chemistry

Type: Award Lecture in Division, Time: FRI 14:30, Chair: Jaeyoung Lee

Accelerating Materials Discovery with Scalable Computations and Machine Learning

Yousung Jung

Korea Advanced Institute of Science and Technology, Korea

Novel materials discovery is a key to addressing many challenges in energy, climate change, and future sustainability. Usual procedure of finding innovative materials based mainly on experiments, however, can take far too long due to a vast and discrete search space, and thus accelerating this process by orders of magnitude using scalable computations would significantly reduce the time and cost of new discovery. In achieving this grand goal, density functional first principles simulation offers a sweet spot between the prediction accuracy and feasibility for most current large scale materials applications. In this lecture, I will talk about some of our recent efforts along this line to understand and design new materials that capture carbon, catalyze CO₂ conversion, and provide storage of that energy. All of these materials are complex, but can also be potentially highly tunable if there is a way to accurately extrapolate the large set of existing data for a new discovery, precisely the area in which the machine learning and artificial intelligence has made waves and significant breakthroughs in recent years. At the end of this talk, thus, I will briefly describe great opportunities in which state-of-the-art computer science techniques in machine learning can contribute greatly to creating solutions to materials problems.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS3-2**

Area: Recent Trend in Surface and Interface Physical Chemistry

Type: Symposium, Time: FRI 15:10, Chair: Jaeyoung Lee

Atomic-scale investigations on single molecules by STM

Hyung-Joon Shin

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

The ability of scanning tunneling microscopy (STM) to probe individual single molecules has enabled revealing material's properties which otherwise would be hidden in the study of an ensemble of molecules. Combining its imaging, manipulation, spectroscopic characterization capabilities, STM has made it possible to achieve single-molecule chemistry. In this presentation, I will introduce some of our STM results on molecular adsorbates on various surfaces, such as insulating films and graphene. On insulating films, the increased life time of vibrationally excited states opens a new dissociation pathway which is not available on metals surface. On graphene surface, fullerene molecules are ordered in a single orientation, resulting from the competition between intermolecular and molecule-substrate interactions. Our results show that the role of supporting substrate is very important for the dynamics and reaction of single molecules on it.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS3-3**

Area: Recent Trend in Surface and Interface Physical Chemistry

Type: Symposium, Time: FRI 15:30, Chair: Jaeyoung Lee

Ongoing studies and instrumentation activities of ambient pressure X-ray photoelectron spectroscopy in Korea Basic Science Institute

Beomgyun Jeong

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

Conventional XPS (X-ray photoelectron spectroscopy) requires ultrahigh vacuum (UHV) for the detection of photoelectrons emanating from a surface. Over the last decade, the development of ambient pressure XPS (APXPS) has made profound impacts on the field of surface science. By allowing gas- and liquid-phase materials in analysis process, it becomes possible to use XPS as a tool for operando spectroscopy in various applications such as gas-phase catalytic reaction and electrochemistry in liquid- or solid-phase electrolyte. This talk will present ongoing studies and instrumentation activities of APXPS in Korea Basic Science Institute (KBSI) that is connected to the linear transfer system for maintaining the sample surface clean in UHV environment from surface preparation to various analyses. A synchrotron X-ray source based APXPS beamline is currently under construction at Pohang Accelerator Laboratory, and its progress status will be presented. Finally, future research plans with the upcoming infra-structure will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS3-4**

Area: Recent Trend in Surface and Interface Physical Chemistry

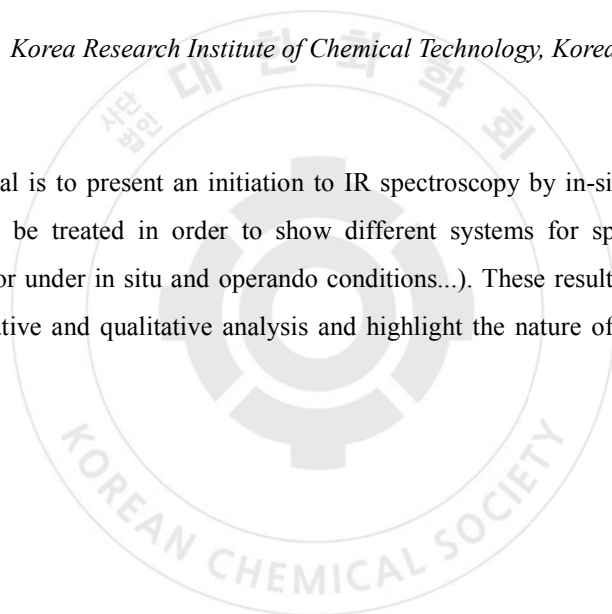
Type: Symposium, Time: FRI 15:50, Chair: Jaeyoung Lee

IR spectroscopy applied to catalysis and adsorption by in-situ and operando system

Ji Woong Yoon, Young Kyu Hwang, Jong-San Chang*

Korea Research Institute of Chemical Technology, Korea

The aim of this practical is to present an initiation to IR spectroscopy by in-situ and operando system. Various examples will be treated in order to show different systems for spectrum acquisition (e.g. temperature, pressure, or under in situ and operando conditions...). These results will be used to present some common quantitative and qualitative analysis and highlight the nature of information that can be obtained.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS3-5**

Area: Recent Trend in Surface and Interface Physical Chemistry

Type: Symposium, Time: FRI 16:10, Chair: Jaeyoung Lee

Direct observation of delayed triplet-state formation through hybrid charge transfer exciton at organic/inorganic interface

Heeseon Lim, Hyuksang Kwon¹, Jeong Won Kim^{1,*}

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

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

Organic/inorganic hybrid solar cell is one of the future generation photovoltaics, which combines organic and inorganic semiconductors by incorporating the merits of either materials. Furthermore, intriguing physical behavior of hybrid “Frenkel-Wannier exciton” at hybrid interface results in unique nonlinear optical properties. [1,2] Therefore, ultrafast charge transport and separation or recombination mechanisms are an important puzzle to be solved out for device efficiency improvement along with each intrinsic material issue. Here, we focus on typical semiconductors, GaAs, as inorganic absorber and C₆₀ or CuPc as organic counterpart. We compare each interfacial electronic structure using ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy. Ultrafast carrier dynamics is studied by using time-resolved two-photon photoemission spectroscopy. Doping type of GaAs and corresponding space charge field control specific charge separation behaviors upon light absorption. While C₆₀/p-GaAs shows electron injection or separation to organic acceptor layer, CuPc/p-GaAs shows hole injection behavior depending on light intensity. Especially, in CuPc/p-GaAs hybrid system, we observe an interesting phenomenon of the delayed triplet-state formation in CuPc. Since direct electron excitation within CuPc is neglected, the delayed triplet state is probably generated via “hybrid charge transfer exciton (HCTE) states”, which is formed by hole injection from GaAs to CuPc. Through the lifetime analysis of HCTE and triplet states, the triplet state turns out to be closely related to high-energy HCTE state. Finally we discuss about hybrid type material design for enhanced charge separation.[1] Phys. Lett. A, 214, 1, (1996), 99.[2] Nat Mater, 12, 1, (2013), 66.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ACBI-10

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Award Lecture in Division, Time: THU 15:25, Chair: Hye Jin Lee

Improvement of MALDI-MS performance for various sample analysis

Jeongkwon Kim

Department of Chemistry, Chungnam National University, Korea

Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) is a fast and versatile technique to obtain the molar mass of a compound, where a laser light is irradiated on the sample target which is normally composed of an analyte and an organic matrix. Due to its ease of operation, fast analysis times, high mass accuracy, and high mass resolution, MALDI-MS is commonly used for rapid analyses of proteins, peptides, synthetic polymers, carbohydrates, and other macromolecules. There are two major drawbacks in MALDI-MS analyses. First, there is almost always interference in the low m/z region, *e.g.*, $< m/z$ 500, due to matrix fragments or its cluster peaks from common matrices. The second drawback is the possibility of inhomogeneity in the distribution of matrix within a MALDI spot. This often leads to poor reproducibility and poor quantitative results. Various efforts have been tried to overcome these drawbacks.

During the presentation, various efforts to improve the performance of MALDI-MS for the analysis of proteins, carbohydrates, lipids, or explosives will be presented. Different matrix materials, additive cations, and additive acids have been tried to analyze small molecules or improve the sensitivity of MALDI-MS. Charcoal could be used as an alternative matrix for the analysis of small molecules. Phosphoric acid was found to be an effective additive for the analysis of peptides with 2,5-dihydroxybenzoic acid matrix. MALDI-MS sample preparation using free-vacuum drying where the matrix-analyte mixture is first frozen and then dried under vacuum, resulted in a homogeneously crystallized matrix-analyte mixture appropriate for quantitative MALDI-MS analysis, improving the reproducibility of MALDI-MS analysis.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ACBI-1**

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 09:00, Chair: Seong Ho Kang

Mechanical bistability of single membrane compartments of live cells

Tae-Young Yoon

School of Biological Sciences, Seoul National University, Korea

Mechanical deformation of cell membranes plays an important role in various cellular tasks. By using magnetic tweezers, we pulled single membrane compartments in cultured living cells. We observed two-state transition in the force-extension curve of single membrane compartment pulling. Our observation indicates that the membrane-skeleton interaction is a central factor for both membrane partitioning and its unconventional mechanical response. I will close the talk by discussing mechanistic insights for a role of this unconventional cell-membrane elasticity in some important cellular processes.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ACBI-2**

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 09:25, Chair: Seong Ho Kang

Overview of single-genome sequencing technologies for lineage tracing of somatic cells

Young Seok Ju

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

All cells that constitute the human body are direct descendants, through a lineage of mitotic cell divisions, of the fertilized egg. During normal mitotic cell division, the genome is replicated with very high, but not absolute, precision, which leads to the incorporation of somatic mutations throughout the course of an individual's life. The somatic mutations then will be inherited to all direct descendants of the specific cell. Therefore, these post-zygotic somatic can be used in lineage tracing as markers if the sequencing accuracy is sufficiently high. In my talk, I would like to overview the acquisition of somatic mutations in human cells, pros and cons of many different single-genome technologies and to discuss genome sequencing strategies in my laboratory which may enable the lineage tracing of many adult human cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ACBI-3**

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 09:50, Chair: Seong Ho Kang

20-nm resolution brain imaging via next-generation expansion microscopy

Jae-Byum Chang

Department of biomedical engineering, Sungkyunkwan University, Korea

The identification and localization of proteins and other biomolecules, throughout entire organs with nanoscale precision would enable many fundamental insights into the mechanisms underlying the operation of normal and pathological biological circuits. We recently discovered that we could physically magnify specimens by embedding them in a dense swellable polymer, anchoring key biomolecules to the polymer mesh, and adding water to swell the polymer, a process we call ‘expansion microscopy’. Despite the high isotropy of the expansion process, the initial polymer recipe enabled just 4-4.5x expansion, or roughly 60-70 nm spatial resolution. Ideally it would be possible to improve the expansion chemistry so as to enable, ultimately, the imaging of membrane boundaries, as well as protein complexes. Here, we report on a next-generation ExM chemistry that can achieve ~15-20x physical magnification of mouse brain tissues, or 20-nm lateral resolution on conventional optical microscopes. As with the first version of ExM, next-generation ExM-processed samples are optically clear. Thus, next-generation ExM may be useful for imaging nanoscale neuronal structures such as synapses over entire neural circuits in intact mammalian tissues. Brain circuit mapping using next-generation ExM may open up a variety of insights into the underpinnings of behavior, cognition, and disease. We continue to refine the chemistry and to explore how affinity tags can be adapted to work in this new expanded environment.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ACBI-5**

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 10:35, Chair: Seong Ho Kang

Automated single-molecule imaging and its applications to cell signaling

Masahiro Ueda

*Graduate School of Frontier Biosciences, Osaka University / Quantitative Biology Center (QBiC),
RIKEN, Japan*

Single-molecule imaging analysis has been applied to living cells and revealed molecular mechanisms of various intracellular events. The techniques have made it possible to directly monitor the behaviors of biomolecules in living cells, in which the locations, movements, turnovers, and complex formations of biomolecules can be detected quantitatively with single molecule sensitivity, providing powerful tools to elucidate molecular mechanisms of intracellular signaling processes. However, technical expertise has been required for both microscope operation and data analysis, which has prevented the analysis from being a standard in medical and biological research. Here, we report a newly developed apparatus for single-molecule imaging analysis in living cells, by which molecules on the plasma membrane can be observed at single-molecule level without manual handling. Cell searching, focusing, and image acquisition were fully automated by utilizing a machine learning method to accomplish high accuracy, efficiency, and reproducibility. Furthermore, immersion-oil feeding, drug dispensing, and setting of the multi-well sample plate containing cells were also automated to observe many cells with different experimental conditions. The apparatus demonstrated that single-molecule imaging of EGF receptors in the living CHO cells were completed for a 96-well plate within one day, in which about 1000 cells were observed and analyzed automatically. Results revealed that EGF receptors adopt multiple states in their diffusion on membrane and undergo the state transition upon EGF stimulations, consistent with previous reports. The working efficiency was dramatically improved, showing that the automatically comprehensive single-molecule analysis in living cells is feasible.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ACBI-6

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 13:30, Chair: Sang-Hee Shim

Breaking the limit by *IRIS*: the merits of fast exchangeable target-binding probes in super-resolution localization microscopy

Naoki Watanabe

Laboratory of Single-Molecule Cell Biology / Department of Pharmacology, Kyoto University Graduate School of Medicine, Japan

I introduce our multi-target super-resolution microscopy, ***IRIS*** (Kiuchi et al. *Nature Methods* 12: 743-746, 2015). While widely acknowledged for 2014 Nobel Prize, an intrinsic problem in super-resolution microscopy had been recognized since late 2000s. According to the Nyquist theorem, structure features smaller than twice the label distances cannot be discerned. Because the antibody is >10 nm wide, this readily limits the resolution of super-resolution microscopy even with super-refined optics. To overcome this problem, ***IRIS*** employs exchangeable fluorescent probes which quickly associate to and dissociate from the target protein. By integrating the centroid position of each single-molecule association event analogously to PALM/STORM, ***IRIS*** yields high-fidelity super-resolved images in fixed specimens. Moreover, ***IRIS*** enables imaging of an unlimited number of targets in the same specimen. It is important to note that ***IRIS*** allows utilization of unlimited 'photons' because fluorescent probes can be added and exchanged during image acquisition. This advantage in 'photon budget' can potentially extend the application of ***IRIS*** in several directions such as 'ultra'-resolution imaging, visualization of multiple components within a narrow area and 3-D super-resolution imaging. ***IRIS*** may thus comprise a useful research and diagnostic platform to elucidate body structure functions. I will present the current development of ***IRIS*** microscopy ongoing in my laboratory as well as several tips in quantitative live-cell fluorescence imaging and single-molecule imaging.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ACBI-7

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 14:10, Chair: Sang-Hee Shim

Iterative antibody reprobng for optical imaging in nano-scale

Sunghoe Chang

Physiology and Biomedical Sciences, Seoul National University, Korea

Despite its enormous usefulness, the current method for simultaneous immunostaining of multiple protein targets requires the primary antibody to be raised in different species, and that the secondary antibodies recognize one of the species exclusively, which put a limit on the number of concurrent visualization of multiple targets. Several SDS-based stripping methods for antibody reprobng have been developed but they suffer from the unavoidable distortion of cellular microstructures and the residual immunoreactivity due to an incomplete removal of antibodies. Here, we develop a new antibody stripping method for optical imaging in nano-scale. We found new method completely striped primary and secondary antibodies off without damaging any cellular structures, allowing us to visualize distinct multiple target proteins sequentially using corresponding multiple primary antibodies regardless of the species, even from the same species. We applied it to the super-resolution stochastic optical reconstruction microscope (STORM). We found iterative STORM imaging unambiguously registered the same locations of undeformed cellular structures with sub-diffraction limit resolution. Furthermore, we applied it for temporal multiplexing with different primary antibodies against distinct target proteins followed by the same Alexa-647 conjugated secondary antibody, and found that iterative STORM imaging with temporal multiplexing clearly visualized five distinct target proteins with subdiffraction resolution without any overlap or mis-localization due to residual antibodies. In summary, we have demonstrated that our method is capable of visualizing multiple biological structures regardless of the species from which the primary antibodies were raised. By combining with temporal multiplexing, this is highly scalable.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ACBI-8**

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 14:35, Chair: Sang-Hee Shim

Single Molecule Nanoparticle Catalysis with Super-resolution Fluorescence Microscopy

JI WON HA

Department of Chemistry, University of Ulsan, Korea

Metal-semiconductor heterostructures are promising visible light photocatalysts for many chemical reactions. However, little is known about the surface active sites and factors that control the catalytic activity and selectivity in these hybrid materials. Here, we use high-resolution super-localization imaging to reveal the nature and photocatalytic properties of the surface active sites on single Au-CdS hybrid nanocatalysts. We find that the excited surface plasmons in the metal play an important role in photocatalysis, and one must consider the photoinduced plasmonic effect together with the facets and defects of the metal. We experimentally reveal two distinct, incident energy-dependent charge separation mechanisms that result in completely opposite photo-generated active sites (e^- and h^+) and divergent energy flows on the hybrid nanocatalysts. Engineering the direction of energy flow at the nanoscale can provide an efficient way to overcome important challenges in photocatalysis, such as controlling catalytic activity and selectivity. These results bear enormous potential impact on the development of better visible light photocatalysts for solar-to-chemical energy conversion.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ACBI-9

Area: [Analytical Chemistry Division - JASIS (Japan) - Life Chemistry Division Joint Symposium] Super-Resolution Optical Microscopy and Single-Cell Analysis

Type: Symposium, Time: THU 15:00, Chair: Sang-Hee Shim

Dark-Field Illumination-Based Enhanced Fluorescence-free 3D Super-Resolution Microscopy

Seong Ho Kang

Department of Applied Chemistry, Kyung Hee University, Korea

Fluorescence-free three-dimensional (3D) super-resolution microscopy (SRM) was developed based on wavelength-dependent dark-field illumination and a least-cubic algorithm. Various plasmonic nanoparticles on a glass slide (i.e., gold nanoparticles, GNPs; silver nanoparticles, SNPs; and gold nanorods, GNRs) were imaged and sliced in the z-direction to a thickness of 10 nm. The 3D coordinates of individual GNP, SNP, and GNR (x, y, z) were resolved by fitting the data with 3D point spread functions using a least-cubic algorithm and collation. Final, 3D SRM images were obtained by resolving 3D coordinates and their Cramér-Rao lower bound-based localization precisions in an image space (530 nm × 530 nm × 300 nm) with a specific voxel size (2.5 nm × 2.5 nm × 5 nm). The least-cubic method was more useful for finding the center in asymmetric cases (i.e., nanorods) with high precision and accuracy compared with the commonly used least-square method. This fluorescence-free 3D SRM technique was also successfully applied to resolve the positions of various nanoparticles in live single cells and nanobiochips with subdiffraction limited resolution in 3D.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL-5

Area: [Analytical Chemistry Division - JASIS (Japan) Joint Symposium] Elemental Analysis Using Plasma Spectroscopy and Mass Spectrometry

Type: Award Lecture in Division, Time: FRI 16:10, Chair: Yonghoon Lee

The Role and Responsibility of the Analytical Chemists in Industry: The Paradigm Shift

Sung-Chan Jo

Display Research Center, Samsung Display Co., Ltd., Korea

Long had it been such that analytical data were just attached as a simple addendum in a report in most industry. The situation was much worse when it comes to a market where micro-to-nanometer scale electronic devices were the major products. In such a company, electron microscopic data were always in the front line of the technical debates and chemical analyses were included better than nothing.

Often times, novel analytical methodologies were believed to come automatically with new instruments and the chemists in the field would choose to switch to R&D positions discarding analytical roles in a firm. That was because the opinion leaders regarded analysis-related issues as not serious nor important in the engineering practices even when they are with chemical businesses. In these types of industry, the researchers and engineers did not rely on analytical reports but simply use them as the back-up information for their own 'proposed mechanisms'. They would even request multiple analyses for the same sample until the very moment when they get what they exactly want. Under such circumstances, analytical chemists would never get any credit for their work in any way. Followers could survive in this fashion whatever the number is; first, second, third.....

However, there has been a spectacular change in the field and companies started to stand off in the front lines in the world. Consultants from developed countries became not so helpful as before since Korean firms now started to take a new materials and processes. In this situation, wide and long experience is not so important as creative conclusion out of profound understanding in the relevant topics.

Nowadays, huge investment has been made in industry to strengthen the analytical capability and the word 'analysis' turned up very popular. The management call for definite clues from analytical chemists, which require the very core extract out of perplexing data. Therefore, analytical chemists confront a new hardship to get credit. In this presentation, questions are raised as to how and what analytical reports are

written not to be treated as addenda, to which a very practical answers are provided. Some of the real world examples are also included to help the audience to understand the detailed situations and how-to.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL-1

Area: [Analytical Chemistry Division - JASIS (Japan) Joint Symposium] Elemental Analysis Using Plasma Spectroscopy and Mass Spectrometry

Type: Symposium, Time: FRI 14:30, Chair: Jong-Ho Park

LA-ICP-MS Analysis for Characterization of Dispersion Fuel

Jeongmook Lee^{*}, JAI IL PARK, Young-Sang Youn, Yeong Keong Ha, Jong-Yun Kim

Korea Atomic Energy Research Institute, Korea

Dispersion fuels with low enriched uranium have been developed as potential fuels for research and test reactors in place of highly enriched uranium fuels that could cause global threat. U-Mo dispersion fuel in which U-Mo fuel particles are dispersed in Al matrix has shown more excellent and stable fuel performance than many dispersion fuel candidates. Many experimental techniques have been used to characterize and analyze U-Mo dispersion fuels. In this study, laser ablation inductively coupled plasma mass spectrometry has been applied to characterize U-Mo dispersion fuel. $^{98}\text{Mo}/^{238}\text{U}$ ratios in U-Mo fuel particle were measured to confirm the uniformity of the Mo/U element ratio. Further line scanning method was also applied to determine the domain size of isotopes. It is concluded that laser ablation inductively coupled plasma mass spectrometry is enough to measure isotope ratios and the dispersed domain of isotopes in U-Mo dispersion fuels simultaneously.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL-2

Area: [Analytical Chemistry Division - JASIS (Japan) Joint Symposium] Elemental Analysis Using Plasma Spectroscopy and Mass Spectrometry

Type: Symposium, Time: FRI 14:50, Chair: Jong-Ho Park

Purification of 4N Gallium by zone refining and trace by Glow discharge mass spectrometer analysis

Jasik Yoon

Division of Advanced materials engineering, ChungNam National University, Korea

Recently, the market demand for high-purity metal is increased and purification method of the gallium high productivity is required. Gallium have low melting point (29.76 °C) and super cooling properties and that property was not applied to zone refining method of the ordinary. Therefore, we produced zone refining system for low melting metal by using Direct Cooling and Indirect heating. Purification of 4N gallium was carried out zone refining process. Depending on the refining process up to 5pass, the trace metal impurities such as B, Al, S, Cr, Fe, Ni and Si decrease 4N to 6N. We adopted GD90(MSI, UK) to the measurement of impurities in high purity Gallium metal for prevent gallium melt. GDMS, especially GD 90 is a powerful analytical method capable of analyzing solid samples without chemical decomposition step and analyzing a low-melting metal by adopting liquid nitrogen cooling and slow sputter method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL-3

Area: [Analytical Chemistry Division - JASIS (Japan) Joint Symposium] Elemental Analysis Using Plasma Spectroscopy and Mass Spectrometry

Type: Symposium, Time: FRI 15:10, Chair: Jong-Ho Park

Surface-Enhanced Laser-Induced Breakdown Spectroscopy for Liquid Analysis

Yonghoon Lee

Department of Chemistry, Mokpo National University, Korea

For liquid samples in small amounts, it is very important to obtain repeated measurements with high precision enough to be accepted for a specific application. Usually, bio-fluid or forensic samples such as blood, urine, etc. are provided for analysis in limited amounts. We devised a laser-patterned silicon wafer (LPSW) substrate to spread a water (or aqueous solution) droplet in the pre-defined region. This makes it possible to get several reproducible measurements for a single droplet sample. By spreading the droplet on the laser-patterned area and drying it, the residues can be distributed very homogeneously. This capability of the LPSW substrate is very useful for the elemental analysis techniques for water droplets using laser-ablation sampling such as laser-induced breakdown spectroscopy (LIBS) and laser-ablation inductively-coupled plasma mass spectrometry (LA-ICP-MS). The relatively more homogeneous distribution of dry residues on the LPSW substrate in comparison with that on the bare silicon wafer substrate was found to be due to enhanced hydrophilic attraction between the water droplet and the substrate surface. The capillary interaction using the laser-produced trenches can be suggested as the underlying mechanism of the enhanced surface hydrophilicity. Also, the higher density of laser-produced trenches on the substrate leads to the larger accumulated emission intensities observed in LIBS spectra. This can be attributed to the higher laser sampling efficiency due to the more homogenous distribution of dry residues that decreases the possibility of missing spots where the residues are concentrated. Performances and applications of this methodology will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL-4

Area: [Analytical Chemistry Division - JASIS (Japan) Joint Symposium] Elemental Analysis Using Plasma Spectroscopy and Mass Spectrometry

Type: Symposium, Time: FRI 15:30, Chair: Yonghoon Lee

Analysis of chemical reactions in the plasma for quantitative underwater laser-induced breakdown spectroscopy

Tetsuo Sakka

Department of Energy and Hydrocarbon Chemistry, Kyoto University, Japan

Laser induced breakdown spectroscopy (LIBS) is a method for spectrochemical analysis of the target materials on the basis of the plasma generation by a pulsed laser irradiation. The method does not require pretreatment of the sample, and can realize elemental analysis of a solid target submerged in water without taking it out from the water. We can expect ranges of applications, in which on-site and in-situ analysis is crucial. Especially, we are interested in the application to deep-sea mineral explorations. In general, the density of atomic species in the plasma is very high due to the confinement effect of water. Therefore, the atomic emission lines are usually very broad, and continuum dominates the spectra, leading to the difficulty in elemental analysis. We have found that a longer pulse, such as the pulse width of 100-ns or so, can avoid the high density of the plasma at the delay time of several hundred nanoseconds to one microsecond from the pulse irradiation, and are successful in observing narrow atomic lines from the laser-induced plasma in water [1]. For LIBS we observe the laser-ablated atomic species in the plasma. For the spectral line intensity to be quantitative as the elemental analysis of the target materials, the elemental composition in the plasma should preserve the target composition. However, after a certain delay from the irradiation, the temperature of the plasma decreases, and this causes the formation of diatomic or larger molecules, which alter the composition of free atomic species. This obviously results in an unwanted alteration of the relative spectral intensities. Therefore, to obtain quantitative results, we have to investigate not only the stoichiometry of the ablation process, but also chemical reactions in the plasma. In the present work, we investigate the time evolution of atomic species in the plasma and in the subsequent bubble. To obtain information of the population densities of atomic species after the plasma quenching, we developed an instrumentation to measure absorption spectra of the species in the bubble after the plasma quenching. It is highly probable that the plasma in

water is in the local thermal equilibrium (LTE) in the sense that electronic excitation temperatures, vibrational and rotational temperatures of diatomic molecules, etc., all agree with each other. This suggests that the chemical reactions are also close to equilibrium. We simulated the densities of chemical species by assuming that they are in the equilibrium, and that the equilibrium changes rapidly by following the rapid decrease of the temperature. Such simulation results explained well the experimental observation of the behavior of the atomic densities in the plasma.[1] T. Sakka et al., Appl. Phys. Lett., 88, 061120 (2006).



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO-4**

Area: Frontiers in Chemical Biology & Protein Chemistry

Type: Award Lecture in Division, Time: FRI 10:15, Chair: Sang Jeon Chung

Structural studies on protein complexes from bacteriophage, flagellum, and divisome

Hyung Ho Lee

Division of Chemistry, Seoul National University, Korea

Atomic structure on protein complexes is crucial for understanding its molecular mechanism. In this talk, I will present structural and functional studies on three protein complexes. In the first part, the structural and functional studies on repressor-antirepressor complex from bacteriophage will be discussed. We showed an uncharacterized mechanism of non-canonical DNA binding and induction by a repressor (Rep) from the temperate Salmonella phage SPC32H; this mechanism was revealed using the crystal structures of homotetrameric Rep (92-198) and a hetero-octameric complex between the Rep and its antirepressor (Ant). The canonical method of inactivating a repressor is through the competitive binding of the antirepressor to the operator-binding site of the repressor; however, these studies revealed several non-canonical features. In the second part, the structural and functional studies on the FliD-FliT complex from Salmonella will be discussed. Bacterial flagellar biogenesis is controlled by a negative feedback loop. When FliD was secreted at the late step of flagellar assembly, the FliD-FliT complex disassembled and free FliT bound to the FlhDC complex, a master regulator of flagellar biogenesis, subsequently inhibiting the overall expression of flagellar proteins. In this study, we analyzed the role of the FliD C-terminal domain in pentamer formation and interaction with FliT. In the third part, the structural and functional studies on the component proteins of divisome will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO-1**

Area: Frontiers in Chemical Biology & Protein Chemistry

Type: Symposium, Time: FRI 09:00, Chair: Jung-Min Kee

Engineered protein assemblies to utilize biomolecular multivalency

Yongwon Jung

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

Multivalency is a key principle in nature for many biological processes such as cell-cell communications, phase separation, and even simple DNA hybridization. For example, multivalent interactions between cells or with other organisms (bacteria and viruses) are governed by multiple ligand-receptor interactions on cell surfaces. Simple (and often weak) individual biomolecular interactions can be highly strengthened and diversified by employing multivalency. To study and employ multivalent bio-interactions, however, multivalent scaffold architectures that can display multivalent biomolecules in a well-defined manner must be developed. Here I will introduce several new strategies to fabricate large protein assemblies, which can be valuable assets to utilize multivalent protein interactions. In particular, modifications and applications of fluorescent proteins, avidin proteins, and cage proteins with highly interesting binding properties will be discussed. Several examples of how newly fabricated protein assemblies can be applied in bioanalytical or biomedical applications will also be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO-2**

Area: Frontiers in Chemical Biology & Protein Chemistry

Type: Symposium, Time: FRI 09:25, Chair: Jung-Min Kee

Genetic incorporation of unnatural amino acids biosynthesized from simple starting materials

HYUNSOO LEE

Department of Chemistry, Sogang University, Korea

The incorporation of unnatural amino acids (UAAs) with novel functional groups into proteins has expanded our ability to study protein structure and function. In this method, most components required to biosynthesize UAA-containing proteins are supplied by host cells into which the plasmids encoding an evolved tRNA/aminoacyl-tRNA synthetase (aaRS) pair and a target protein are introduced. The only additional component required is a UAA, which should be supplied in the growth medium. Many of these UAAs are expensive, and most of the biochemically interesting UAAs are not commercially available and have to be prepared via multistep synthesis. Therefore, new, less expensive and labor-intensive technologies for supplying UAAs to host cells are in demand, especially in a large-scale protein expression for pharmaceutical or industrial applications. In this study, UAAs were biosynthesized by heterologous enzymes from simple starting materials, and the UAAs were directly incorporated into proteins in bacterial cells. This direct incorporation system showed efficient UAA incorporation with no incorporation of any natural amino acid and comparable protein yields with the genetic incorporation system using UAAs. In addition, biochemical applications of mutant proteins containing UAAs biosynthesized by this system showed its potential for protein conjugation and a large scale protein production for pharmaceutical and industrial applications. Finally, this work would provide an impetus for expansion of biosynthesis of unnatural amino acids to more challenging and interesting amino acids.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO-3**

Area: Frontiers in Chemical Biology & Protein Chemistry

Type: Symposium, Time: FRI 09:50, Chair: Jung-Min Kee

Mitochondria Localization-induced Self-Assembly for New Cancer Therapy

Ja-Hyoung Ryu

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

Self-assembled structures in Nature play essential roles in living systems, such as, in protein folding and the formation of biological membranes. The formation of most biological nanostructures is driven by self-assembly processes and the structured biomaterials have biochemical activities such as enzyme activity and protein signaling. The artificial assembly of synthetic building units inside a living cell and the interaction of these units with the cellular components have rarely been studied, but are emerging as an intriguing strategy to control cellular fate. In particular, self-assembly inside cellular organelles is challenging because of the practical difficulty in observing the complex intracellular environment, and thus has not yet been reported. Achievement of artificial self-assembly of small molecules inside such organelles could be an advanced strategy for an efficient external control over organelle function and manipulation of the cellular fate. Considering the role of vicious mitochondrial fibril proteins such as amyloid beta (A β) in Alzheimer's disease, we hypothesized that artificial induction of fibril formation inside the mitochondria could promote mitochondrial dysfunction and induce cell damage. Amphiphilic peptides with a mitochondrial targeting unit selectively accumulate in the mitochondria and self-assemble into an ordered structure because inside the confined organelle, the concentration of the peptides is significantly increased over their critical aggregation concentration. The fibrous structure inside the mitochondria then disrupts the mitochondrial membrane to cause leakage of the mitochondrial contents into the cytosol, resulting in severe damage to the cells. The high negative membrane potential of mitochondria in cancer cells increased the accumulation of Mito-FF, which resulted in selective supramolecular assembly in the cancer cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGNI-1**

Area: Current Trends in Organic Chemistry I: Unexpected Reactivity and Selectivity

Type: Award Lecture in Division, Time: THU 13:00, Chair: Woo-Dong Jang

Development of synthetic methods using decarboxylative coupling of alkynoic acids

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 Sonogahsira type coupling of terminal alkyne showed similar reactivity in most cases, the unique reactivity of alkynoic acid has been found in the multicomponent reactions including metal-free reactions.

In this presentation, we would like to discuss some of our recent research progress towards the decarboxylative coupling reactions of alkynoic acids.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGNI-2**

Area: Current Trends in Organic Chemistry I: Unexpected Reactivity and Selectivity

Type: Symposium, Time: THU 13:30, Chair: Kyungsoo Oh

Total Synthesis of Natural Products via Nitrogen-to-Carbon Chirality Transfer

Sanghee Kim

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

A chirality transfer method for the asymmetric synthesis of α -quaternary amino acid derivatives will be discussed. The high diastereoselectivity in the N-quaternization was achieved via the control of stereodynamics of proline. The generated N-chirality of quaternary ammonium was transferred back to the α -carbon chirality via stereospecific reactions (N \rightarrow C chirality transfer) to give α -quaternary prolines. This new strategy was applied in a straightforward manner to the total synthesis of alkaloid natural products.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGNI-3**

Area: Current Trends in Organic Chemistry I: Unexpected Reactivity and Selectivity

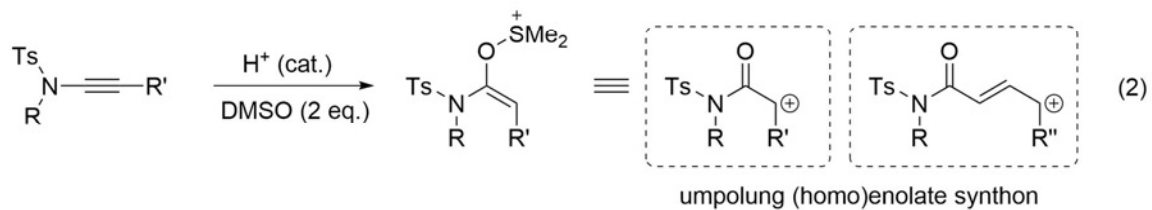
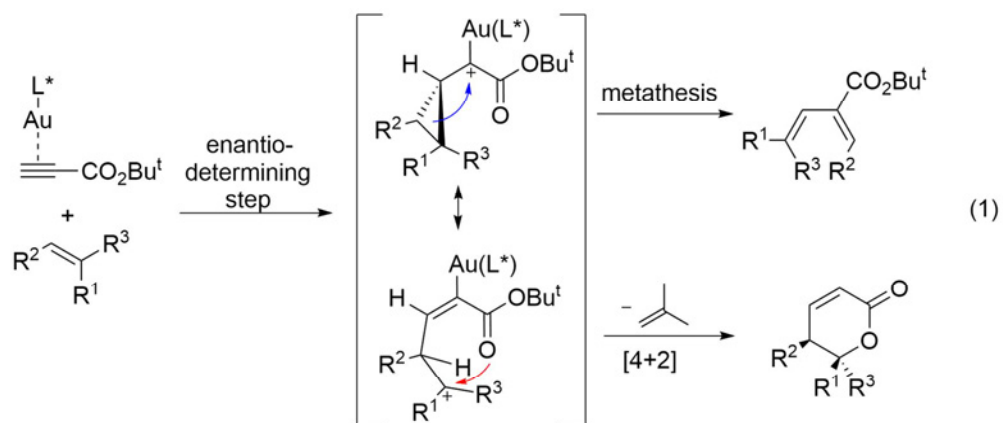
Type: Symposium, Time: THU 14:00, Chair: Kyungsoo Oh

Engaging Alkynes under Metal- and Non-Metal Catalysis

Seunghoon Shin

Department of Chemistry, Hanyang University, Korea

Proper analysis and identification of reaction intermediates in catalysis often leads to new reaction discoveries. In this presentation, I will describe some of our recent investigations in asymmetric gold catalysis as well as Brønsted acid catalysis. Despite remarkable advances in gold catalysis during the last decade, there is only a few intermolecular reactions, especially in an enantioselective sense.¹ In the reaction between alkynes and alkenes, enantio-determining step involves discrimination of prochiral face of the olefin nucleophile, approaching away from the linearly coordinated gold complex (Eq. 1).^{2a} After extensive efforts, we found that 1,1,2,2-tetrachloroethane and AgNTf₂ as the optimal combination of solvent and counter-anion. Although 80~98%ee was achieved, some substrates gave a lower yield of [4+2] product, due to the unwanted formation of metathesis and conjugate addition product. Serendipitously, we found that addition of SDS surfactants significantly suppressed these side pathways, allowing an efficient access to diverse α,β -unsaturated- δ -lactones.^{2b,c} Organocatalytic activation of C-C multiple bonds are much less common than C=N or C=O activation. In this vein, ynamide derivatives are a special class of alkynes that can be activated by Brønsted acids. Recently, we have uncovered acid-catalyzed oxidation of ynamides can be achieved with pyridine-N-oxide or dimethyl sulfoxide as terminal oxidants, emulating a carbene reactivity.³ This umpolung approach allows bimolecular coupling of a wide range of nucleophiles, which is otherwise difficult to achieve.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN1-4

Area: Current Trends in Organic Chemistry I: Unexpected Reactivity and Selectivity

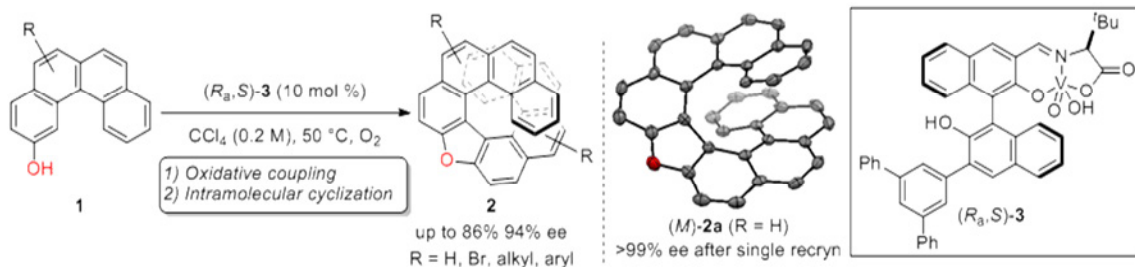
Type: Symposium, Time: THU 14:45, Chair: Kyungsoo Oh

Enantioselective Carbon-Carbon Bond-forming Reactions Catalyzed by Vanadium(V) Complexes

Shinobu Takizawa*, Makoto Sako, Hiroaki Sasai

The Institute of Scientific and Industrial Research, Osaka University, Japan

Optically active helicenes and other related helical molecules have received considerable attention due to their high potential as catalysts, liquid crystals and molecular devices. However, efficient enantioselective synthetic method of helicenes, in particular, oxahelicenes, is rather limited. Herein, we report a vanadium catalyzed enantioselective domino oxidative coupling/intramolecular cyclization of polycyclic phenol **1**.¹ The vanadium complex (*R_a,S*)-**3** works as a redox² and Lewis acid catalyst³ to promote this sequential reaction to give oxa[9]helicenes **2** in up to 86% yield and 94% ee. The enantiopure **2a** (R = H) was readily obtained by a single recrystallization of the product and the absolute configuration of resulting **2a** was determined to be (*M*)-form by X-ray crystallographic analysis. In this presentation, the first regio- and enantioselective oxidative coupling of hydroxycarbazoles⁴ and monocyclic phenols will also be discussed. [References] 1) Sako, M.; Takeuchi, Y.; Tsujihara, T.; Kodera, J.; Kawano, T.; Takizawa, S.; Sasai, H. *J. Am. Chem. Soc.* **2016**, *138*, 11481. 2) Kim, H. Y.; Takizawa, S.; Sasai, H.; Oh, K. *Org. Lett.* **2017**, *19*, 3867. 3) Takizawa, S.; Arteaga, F. A.; Yoshida, Y.; Kodera, J.; Nagata, Y.; Sasai, H. *Dalton Trans.* **2013**, *42*, 11787. 4) Sako, M.; Ichinose, K.; Takizawa, S.; Sasai, H. *Chem. Asian J.* **2017**, *12*, 1305.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGNI-5**

Area: Current Trends in Organic Chemistry I: Unexpected Reactivity and Selectivity

Type: Symposium, Time: THU 15:15, Chair: Kyungsoo Oh

Site-Selective Catalytic C-H Functionalization: Design, Synthesis and Biological Evaluation of Novel Heterocycles

IN SU KIM

School of Pharmacy, Sungkyunkwan University, Korea

With considerable progress in medicinal chemistry, the construction of heterocycles has received increasing attention in the past decades. In particular, N-heterocycles such as indoles, indolines, indazoles, and cinnolinones are widely found to be biologically relevant scaffold in natural products, pharmaceuticals, agrochemicals, and functional materials. Therefore, the directing group-assisted N-heterocycles synthesis via C-H bond activation is highly attractive in pharmaceutical industry. Thus, we recently focused the construction of other N-heterocycles via tandem C-C and C-N bond formations followed by intramolecular cyclization. Moreover, our groups recently reported the synthesis and biological evaluation of novel heterocyclic molecules through Rh(III)-, Ru(II)- and Ir(III)-catalyzed C-H functionalizations of biologically relevant isoindolinones, xanthenes, chromones, indolines, and etc. We herein describe a brief summary of our recent works and present progress works on the synthesis and biological evaluation of heterocycles through Rh(III)-catalyzed C-H functionalization. Notably, we present the unexpected reactivity and selectivity on Rh(III)- and Ru(II)-catalyzed C-H functionalizations leading to the discovery of alternative reaction pathways.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN2-1**

Area: Current Trends in Organic Chemistry II: Organic Materials & Supramolecular Chemistry

Type: Symposium, Time: FRI 09:00, Chair: Won-jin Chung

Bispecific Antibody Conjugates for Cancer Immunotherapy

Chan Hyuk Kim

Department of Life Science, KAIST, Korea

Cancer immunotherapy has been drawing growing attention as a novel promising therapeutic modality for cancer. Unlike conventional chemo- or radiotherapy, immunotherapy treats cancer by unleashing the suppressed activity of the patient's own immune system and harnessing its power to fight cancer, to achieve robust anti-tumor responses while minimizing collateral damages to normal tissues. Among several immunotherapeutic approaches, T cell-based immunotherapeutics such as bispecific antibodies and chimeric antigen receptor (CAR) T cells have generated unprecedented responses in clinics, and have become promising therapeutic modalities for the treatment of refractory cancers. In this talk, I will briefly discuss our recent efforts on developing novel approaches for T cell-based immunotherapeutic using novel bispecific antibody conjugates, in particular PSMA-targeting small molecule antibody conjugate and switchable CAR-T platform.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN2-2**

Area: Current Trends in Organic Chemistry II: Organic Materials & Supramolecular Chemistry

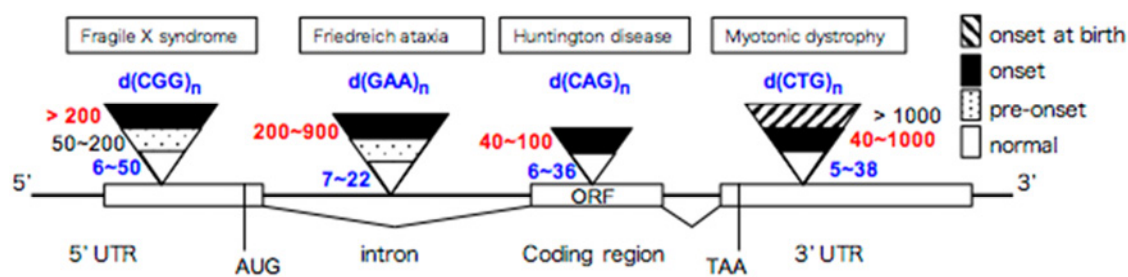
Type: Symposium, Time: FRI 09:25, Chair: Won-jin Chung

Targeting Diseases-related Trinucleotide Repeat Sequences by Small Organic Molecules

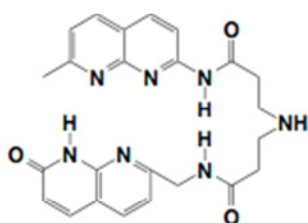
Kazuhiko Nakatani

The Institute of Scientific and Industrial Research, Osaka University, Japan

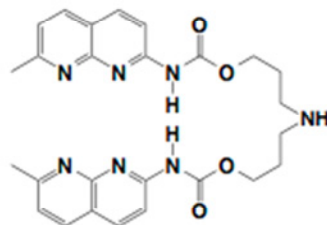
The expansion of trinucleotide repeat (TNR) sequences in human genome is known as causatives of more than 40 hereditary neurological disorders. The CAG sequence in the coding region of protein huntingtin for the patients of Huntington disease is 40~100 repeats, whereas that is about 6~36 repeats for healthy individuals. Aberrant and enormous expansion of the CTG sequence of 5~38 repeat in 3'-UTR of DMPK gene up to 40~1000 repeats was observed for the patients of Myotonic Dystrophy type 1. The CGG repeat expansion causes the Fragile X syndrome upon expansion up to more than 200 repeats. The common feature of the mechanism in TNR expansion and contraction involves the non-canonical secondary structures produced on the TNR sequences. The expanded CXG repeats can fold into a hairpin secondary structures containing a number of the palindromic CXG/CXG motif, which hold a X-X mismatch flanked by two C-G base pairs. We have discovered small molecules that selectively bound to the CAG/CAG motif, CGG/CGG motif, and other repeat sequences. In the presentation, we will describe and discuss our recent progress on these studies.



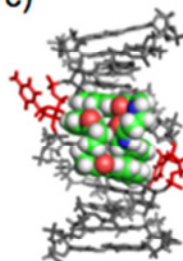
a) NA



b) NCD



c)



The relation of representative trinucleotide repeat and diseases and molecules binding to the repeat



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN2-3**

Area: Current Trends in Organic Chemistry II: Organic Materials & Supramolecular Chemistry

Type: Symposium, Time: FRI 10:00, Chair: Won-jin Chung

Chemical Posttranslational modification of Proteins: C-C bond formation reaction using radical chemistry

hee-yoon lee

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

Posttranslational modification of proteins expand the diversity of protein function (Scheme 1).¹ Though development of C-C bond forming reaction with proteins is important in studying the posttranslational modification of proteins, due to aqueous nature of the reaction medium hindered the development of C-C bond forming reaction. Only handful examples of such reactions have been reported with limited applicability.² Free radicals are well known reactive intermediates in the C-C bond formation and widely used in organic synthesis. Another advantage of free radicals in addition to the high reactivity is the compatibility with water.³ Unlike other reactive intermediates, radicals do not react with water molecules and thus the radical reaction can be run in aqueous medium. That could allow development of organic reactions with proteins. To mimic posttranslational modification of nature, we have devised a reaction protocol using radical C-C bond forming reaction using dehydroalanine as the common precursor. Development of the C-C bond forming reaction with dehydroalanine in water and application of the reaction to the modification of proteins will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN2-4

Area: Current Trends in Organic Chemistry II: Organic Materials & Supramolecular Chemistry

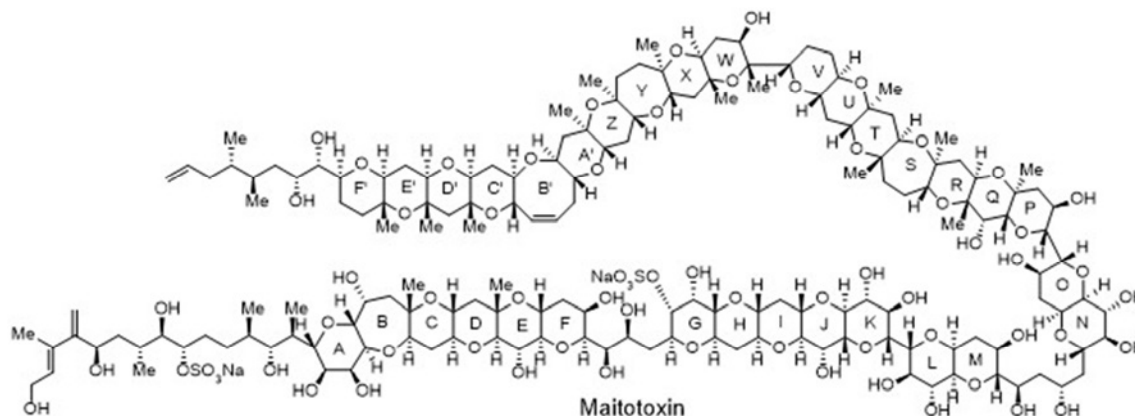
Type: Symposium, Time: FRI 10:25, Chair: Won-jin Chung

Structure-Activity Relationship Studies of Maitotoxin Based on Chemical Synthesis of Partial Structures

Tohru Oishi

Department of Chemistry, Graduate School of Scienc, Kyushu University, Japan

Maitotoxin (MTX) was first discovered as one of the toxins responsible for ciguatera seafood poisoning and later found to be a product of the epiphytic dinoflagellate *Gambierdiscus toxicus*. MTX is one of the largest non-biopolymer (MW 3422) and most toxic against mammals (50 ng/kg) known to date. MTX elicits remarkable biological activities at extremely low concentration, for instance, hemolysis (15 nM) of red blood cells and calcium ion influx (0.3 nM) in all cell types examined to date. Despite a large number of pharmacological and biophysical investigations, the precise mode of action of MTX has not been elucidated at the molecular level, primarily due to the limited availability of MTX from natural sources. As a part of the structure-activity relationship studies of MTX based on the chemical synthesis of partial structures of MTX, the C'D'E'F', WXYZA'B'C', QRS, NOPQR(S), and LMNO ring systems were synthesized. By using these fragments, inhibitory activity against MTX-induced calcium ion influx was evaluated.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN3-1**

Area: Current Trends in Organic Chemistry III: New Reactions and Methodology

Type: Symposium, Time: FRI 14:30, Chair: Jung Woon Yang

Development of PET radiotracers for Neurobiological Targets

Sun-Joon Min

Department of Chemical & Molecular Engineering, Hanyang University, Korea

Serotonin (5-HT) is a major excitatory neurotransmitter that plays an important role in normal physiological conditions. They are mediated by multiple receptor subtypes that have been classified into seven subfamilies (5-HT₁₋₇). Among them, the 5-HT_{2C} is widely distributed in the human brain, in particular, displaying a high density in striatal, cortical, and limbic regions. It has been reported that dysfunction of the 5-HT_{2C} contributed to a variety of brain-related disorders such as schizophrenia, Parkinson's disease, and anxiety. Up to date, it is difficult to study a direct mechanism of action between the 5-HT_{2C} and such brain diseases due to lack of proper chemical probes. Accordingly, development of an in vivo method for measuring its function and density is important to identify the role of the 5-HT_{2C} receptor in the brain. Thus, PET imagining might be one of the potential tools for this purpose. A number of selective 5-HT_{2C} ligands have been developed, but only a few of them have been evaluated as PET radiotracers. Herein, we describe synthesis and biological evaluation of a pyrimidine derivative as a selective 5-HT_{2C} PET radiotracer. We have successfully developed a synthetic route toward [¹⁸F]-labeled pyrimidine derivative through late-stage fluorination reaction using an arylodonium tosylate as a key intermediate. The in vivo evaluation of this selective PET radioligand in normal rats indicated that our PET radiotracer exhibits a high level of specific binding to 5-HT_{2C} receptors in the rat brain.

Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: **ORGN3-2**

Area: Current Trends in Organic Chemistry III: New Reactions and Methodology

Type: Symposium, Time: FRI 15:00, Chair: Jung Woon Yang

Development of Transient Ligands for Palladium-catalyzed sp^3 C-H Bond Arylation

Hyojin Park, Kwangho Yoo, Byunghyuck Jung^{1,*}, Min Kim^{*}

Department of Chemistry, Chungbuk National University, Korea

¹*School of Basic Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Directing groups are essential part for regio-selective transition metal-catalyzed organic reactions. Generally, the first step of transition metal-catalyzed reaction is the formation of coordination bond between directing groups and metal ion (or cluster). However, this directing group approach typically requires the additional steps for the installation and removal of the chelating component, and diminishes the efficiency and compatibility of the reactions in the practical concept. Recently, C-H bond activation reactions using temporary, transient directing groups that can be reversibly linked to the substrate have studied to overcome this issue.^[1-3]

In this presentation, our recent results about transient ligand developments for palladium-catalyzed C-H bond activation, especially sp^3 C-H arylations will be discussed. The novel amino acid and amino alcohol-based transient directing group reversibly reacts with the aldehydes in the substrate to imine formation. And the palladium catalyst could be positioned, and the inert C-H bond activation and arylation are performed. The preparation of new ligands and their catalytic activities will be presented along with substrate scopes for sp^3 C-H bond arylation reactions.

References

- [1] Zhang, F.-L.; Hong, K.; Li, T.-J.; Park, H.; Yu, J.-Q. *Science*, 2016, 351, 252.
- [2] Ma, F.; Lei, M.; Hu, L. *Org. Lett.* **2016**, 18, 2708.
- [3] Liu, X.-H.; Yu, J.-Q. et. al. *J. Am. Chem. Soc.* **2017**, 139, 888.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN3-3**

Area: Current Trends in Organic Chemistry III: New Reactions and Methodology

Type: Symposium, Time: FRI 15:30, Chair: Jung Woon Yang

Biosynthetically Inspired Total Syntheses of Complex Natural Products

Sunkyu Han

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

Despite an extensive history of natural products total synthesis, devising efficient synthetic strategies for complex secondary metabolites is still intellectually daunting and toilsome. As one means to facilitate the retrosynthetic endeavor, chemists have sought inspiration from the biosynthesis of natural products. We show how structural analysis of biosynthetically relevant natural products and the biosynthetic hypothesis of structurally relevant secondary metabolites can provide hints for the design of synthetic routes. We showcase the viability of this general approach by presenting total syntheses recently completed in our laboratory.¹ References¹. (a) Jo, D.; Han, S. *Org. Chem. Front.* 2017, 4, 506. (b) Jeon, S.; Han, S. *J. Am. Chem. Soc.* 2017, 139, 6302. (c) Kang, T.; Jo, D.; Han, S. *J. Org. Chem.* 2017, ASAP.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN3-4**

Area: Current Trends in Organic Chemistry III: New Reactions and Methodology

Type: Symposium, Time: FRI 16:00, Chair: Jung Woon Yang

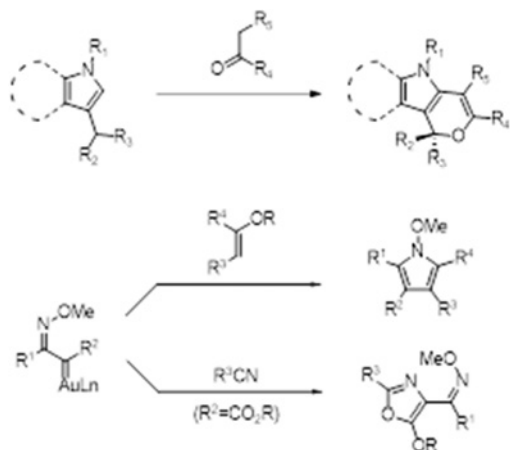
Construction of Scaffold Diversity in Heterocycle Synthesis

Cheol Min Park

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

The development of efficient synthesis of structurally complex heterocycles emerges as an important agenda owing to their utility in many areas including medicine and materials. This talk will describe our recent efforts toward method development for construction of various heterocyclic scaffolds.[1,2] 1) Tandem cross-dehydrogenative cross coupling followed by intramolecular annulation. 2) Divergent reactivity of α -imino carbenes toward unreactive nucleophiles for heterocycle synthesis. In the first part, an efficient synthesis of indolopyrans and pyrrolopyrans based on tandem cross-dehydrogenative coupling followed by annulation will be presented. Cross-dehydrogenative coupling reaction offers broad advantages including obviating prefunctionalization of coupling partners and environmentally friendly conditions. Substantial increase in molecular complexity can be further achieved by combination with subsequent transformations in a tandem fashion. As such, tandem cross-dehydrogenative coupling followed by intramolecular annulation is deemed as a powerful approach to build molecular complexity for heterocyclic scaffolds. Nevertheless, the design of substrates and compatibility of reaction conditions pose significant challenges in the development of tandem reactions. Iodine-mediated reactions have drawn a renewed attention due to its versatile reactivity, benign environmental impact, and more economical processes. Furthermore, the demands for transition metal-free reactions from the pharmaceutical industry calls for the development of alternative reaction conditions. The synthetic method presented today allows the formation of highly substituted indole- and pyrrole-fused pyrans. Examination of substrates with various functionalities has been performed to establish the efficiency and selectivity of the reaction. In order to shed light on the reaction mechanism, several reactions designed to identify putative reactive species and intermediates have been performed. The second part will describe our efforts to identify catalysts that form α -imino carbene-metal complexes with enhanced reactivity leading to the coupling of weak nucleophiles including enol ethers and nitriles. The diverse reactivity of the carbene complexes

allowed us to develop highly efficient synthesis of pyrroles and oxazoles from common substrates depending on coupling partners.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI-1**

Area: Recent Drug Discovery Research in Academia and Industry: Some Success Stories

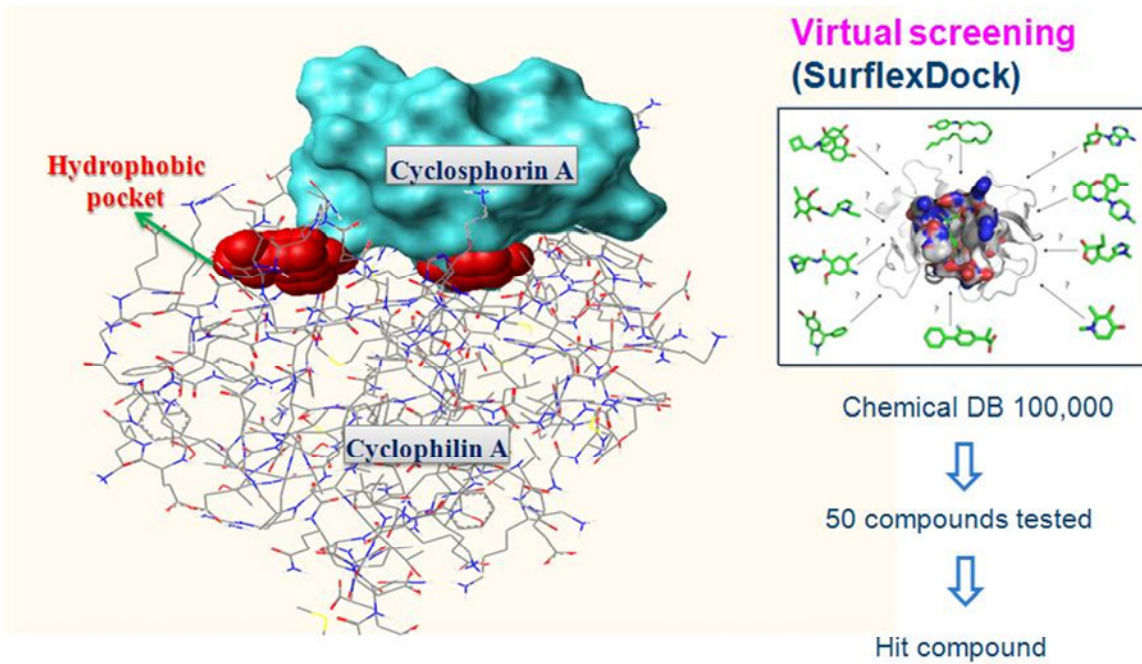
Type: Symposium, Time: THU 13:30, Chair: Taeho Lee

Development of Novel Cyclophilin A Inhibitors for the Treatment of Hepatitis C Virus Infections Based on Structure-based Drug Design

WON JEA CHO

College of Pharmacy, Chonnam National University, Korea

Hepatitis C virus (HCV) is a major cause of end-stage liver diseases. Current therapy relies upon a combination of direct acting antiviral (DAA) with IFN-alpha and ribavirin, but is associated with increased drug resistance and toxicity. The development of host-targeted antiviral agents have predominantly focused on the CypA inhibitors. Despite the successes, the improved CypA inhibitor is still needed to overcome the side effects of CsA-based inhibitors. We performed receptor-based virtual screening (VS) to identify a totally new chemical scaffold, WJCPA-126. Here, we report that WJCPA-126 is a novel CypA inhibitor devoid of immunosuppressive effect. Contrary to CsA and its analogues, the compound showed specific and high binding affinity to CypA and effectively inhibited HCV replication with no acute toxicity in vitro and in vivo. Also, it restored interferon- α (IFN- α) signaling pathway and suppressed interleukin-8 (IL-8) production. Therefore, WJCPA-126 represents a novel CypA inhibitor that has significant potential to extend the therapeutic reach against HCV.



PDB # : 1CWA



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI-2**

Area: Recent Drug Discovery Research in Academia and Industry: Some Success Stories

Type: Symposium, Time: THU 13:55, Chair: Taeho Lee

Fragment-Based Design of Kinase Inhibitors to Override Drug Resistance

Sungwoo Hong

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

More than 500 kinases are encoded in the human genome. Kinase structures present a highly conserved catalytic domain that shares a common cofactor ATP and a Mg ion in a deep cleft. The recent availability of three-dimensional structural information for many kinases has offered opportunities for the development of selective kinase inhibitors based on structural analysis. Two case studies to override point mutations will be presented at the seminar. Although the constitutively activated break-point cluster region-Abelson (BCR-ABL) tyrosine kinase was well known to be responsible for chronic myelogenous leukemia (CML), the existence of drug-resistant mutants of BCR-ABL has made it difficult to develop effective anti-CML drugs. We address the structural features relevant to the stabilizations of the identified inhibitors in the ATP-binding sites. Secondly, identification of new generation EGFR inhibitors against the d746-750/T790M/C797S mutation will be discussed. A number of nanomolar inhibitors were identified using 2-aryl-4-aminoquinazoline as the molecular core and the modified binding energy function involving a proper dehydration term, which provides important structural insight into the key principles for high inhibitory activities against the d746-750/T790M/C797S mutant. Furthermore, some of these EGFR inhibitors showed a greater than 1000-fold selectivity for the d746-750/T790M/C797S mutant over the wild type as well as nanomolar activity against the mutant.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI-3**

Area: Recent Drug Discovery Research in Academia and Industry: Some Success Stories

Type: Symposium, Time: THU 14:20, Chair: Taeho Lee

Development of a novel 11 β -hydroxysteroid dehydrogenase type 1 inhibitor for the potential treatment of type 2 diabetes

Je Ho Ryu, Hyeung-geun Park^{1,*}

Department of Open Innovation, Huons, Korea

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

11 β -Hydroxysteroid dehydrogenase type 1 (11 β -HSD1) is a key enzyme that acts as an NADPH-dependent reductase and converts inactive cortisone into active cortisol, which is an actual circulating glucocorticoid in humans. 11 β -HSD1 is highly expressed in several specific tissues, such as the liver, adipose, and brain. Therefore, 11 β -HSD1 regulates the tissue-specific glucocorticoid levels. Elevated levels of glucocorticoids in the liver and adipose tissue can lead to glucose intolerance, insulin resistance, enhanced hepatic gluconeogenesis, and increased lipolysis. Due to the close relationship between glucocorticoids and metabolic disease risk factors, 11 β -HSD1 inhibition has been regarded as a potential strategy for the treatment of metabolic syndrome and type 2 diabetes. To develop a novel 11 β -HSD1 inhibitor for the potential treatment of type 2 diabetes, high throughput screening of an in-house compound library was performed, and an initial hit compound, N-cyclohexyl-6-(piperidin-1-yl)picolinamide was identified. Based on the docking results, structural modifications were performed as hit-to-lead program and resulted in a significant improvement of both the potency and pharmacokinetic (PK) profiles. The selected lead compound, N-((E)-5-hydroxyadamantan-2-yl)-6-((R)-2-methyl-4-(4-(methylsulfonyl)phenyl)piperazin-1-yl)picolinamide was efficacious in a mouse ex vivo pharmacodynamic (PD) model and reduced the blood glucose, LDL cholesterol, and triglyceride levels in ob/ob mice after oral dosing. Despite its high potency and significantly improved PK/PD profile, this lead compound exhibited moderate-to-strong inhibitory activity against hERG channel and CYP3A4. In order to diminish the hERG and CYP liability, we planned to decrease the lipophilicity of the molecule by introducing a more polar moiety to the left-hand side or replacing the central pyridine ring with a pyrimidine ring. The optimized compound, 2-((R)-4-(2-fluoro-4-(methylsulfonyl)phenyl)-2-methylpiperazin-1-yl)-N-((E)-5-hydroxyadamantan-2-yl)pyrimidine-4-carboxamide (SKI2852) was

identified as a potent and selective inhibitor of 11β -HSD1 with an improved hERG profile and no CYP and PXR liabilities. SKI2852 also exhibited excellent PK profiles across species and highly potent and sustainable PD activity which was three times superior to that of the lead compound. Finally, SKI2852 significantly reduce the blood glucose and HbA1c levels, and improved the lipid profiles in ob/ob mice after oral administration. Moreover, these efficacies were synergistically enhanced by combination with metformin. SKI2852 was selected as a preclinical candidate for GLP compliant toxicological studies and expected to be developed as a novel anti-diabetic drug through clinical trials.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI-4**

Area: Recent Drug Discovery Research in Academia and Industry: Some Success Stories

Type: Symposium, Time: THU 14:45, Chair: Minsoo Song

Identification of new small molecules for metabolic disease

JIN HEE AHN

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

Obesity is a global public health problem. The obesity epidemic has been growing in developed nations, including the United States, for decades. Moreover, this epidemic has spread to developing nations. The worldwide burden is estimated at 1.5 billion overweight and 500 million obese individuals. The negative consequences of obesity have been quantified as exceeding those of either alcohol abuse or smoking. Overweight and obesity constitute the fifth leading risk for global deaths. In June 2013, the American Medical Association officially recognized obesity as a disease. The worldwide explosion of obesity has resulted in an ever-increasing prevalence of type 2 diabetes—a noncommunicable disease that affects more than 370 million people. Without concerted efforts to address the pathogenesis and treatment of this syndrome, the harmful macrovascular and microvascular outcomes of type 2 diabetes will remain a major burden for decades to come. Although several anti-diabetes and obesity drugs are in markets, global pharmaceutical companies and research groups are concentrating their effort on developing more efficacious and safe drugs. In this seminar, discovery of anti-diabetic/obesity agents at GIST and KRICT and their licensing efforts will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI-5**

Area: Recent Drug Discovery Research in Academia and Industry: Some Success Stories

Type: Symposium, Time: THU 15:10, Chair: Minsoo Song

Targeted protein degradation for the next small molecule therapeutics

Jong Yeon Hwang

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

Protein homeostasis in cells is mainly regulated by the ubiquitin-proteasome pathway. This process occurs in a stepwise manner through an enzymatic cascade E1, E2, E3 ubiquitin ligase enzymes, then undergoes proteosomal degradation. Recently, a new and powerful technology called "proteolysis targeting chimeras" (PROTAC) has been actively applied in the field of drug development. Treatment of PROTAC molecule, which contains a ligand for the targeted protein, a ligand for E3 ubiquitin ligase binding, and a linker for connection of two ligands, successfully induced targeted protein degradation, thereby inhibiting cancer growth in in vivo animal model study [1-3]. In this presentation, the recent advances in targeted protein degradation will be introduced and also our recent efforts will be discussed. References [1]. D. P. Bondeson, A. Mares, and C. M. Crews, *Nat. Chem. Biol.* 2015, 11, 611. [2]. G. E. Winter, D. L. Buckley, J. Paulk, J. M. Roberts, A. Souza, S. Dhe-Paganon, J. E. Bradner, *Science*, 2015, 348(6241), 1376. [3]. A. C. Lai, C. M. Crews, *Nat. Rev. Drug Discov.*, 2017, 16, 101.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT1-1**

Area: Synthesis and Application of Two-Dimensional Materials

Type: Symposium, Time: FRI 09:10, Chair: Hyeon Suk Shin

Toward Molecular Designing on Nano-materials for Catalytic Applications

Sungjin Park

Department of Chemistry, Inha University, Korea

During the last half decade, carbon-based nano-materials have been studied in the wide range of applications, due to its excellent electrical, mechanical, and thermal properties as well as good tolerance for chemical modification. Revealing chemical structures of the carbon-based nano-materials is highly important to understand materials properties and to develop optimized processing. This understanding enables us to make new molecular/nano hybrids, which showed interesting performances for catalytic applications. Chemical designing on nano-materials in molecular level would be a promising route to create new hybrid materials and to control various properties of nano- and molecular materials. Organometallic compounds have been a center of molecular catalysts with preeminent catalytic activity and selectivity in a wide range of chemical transformations. Hybridization of organometallic complexes with graphene-based materials can give rise to enhance catalytic performances. In this presentation, I will discuss my recent research activities on the fundamental chemistry of carbon-based nano-materials as well as catalytic applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT1-2**

Area: Synthesis and Application of Two-Dimensional Materials

Type: Symposium, Time: FRI 09:35, Chair: Hyeon Suk Shin

Ultracapacitive Energy Storage Using 2D Nanomaterials Under Extreme Conditions

Ho Seok Park

Department of Chemical Engineering, Sungkyunkwan University (SKKU), Korea

With increasing demand for high performance energy storage devices, the feasibility of reliable and functional energy storage devices that well operates under extreme conditions is of prime importance for expanding applicative fields as well as for understanding materials' intrinsic and extrinsic properties and device physics. In this talk, I will introduce the control in the physical structure and chemical composition of 2D nanomaterials for ultracapacitive energy storage devices under limited circumstances, where conditions are classified into thermodynamic (e.g. pressure, volume and temperature) and kinetic (e.g. high rate and frequency) variables. In addition, a fundamental foundation via in-situ spectroscopic techniques will be presented to understand charge storage phenomenon of new materials and devices occurring on a nanoscale under various circumstances.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT1-3**

Area: Synthesis and Application of Two-Dimensional Materials

Type: Symposium, Time: FRI 10:00, Chair: Hyeon Suk Shin

2D Nanosheets of Layered Metal Compounds: Efficient Building Blocks for Functional 3D Nanohybrids

Seong-Ju Hwang

*Center for Hybrid Interfacial Chemical Structure (CICS), Department of Chemistry and Nanoscience,
Ewha Womans University, Korea*

The exfoliated 2D nanosheets of layered metal compounds attract intense research interest because of their unique physicochemical properties and useful functionalities. The 2D inorganic nanosheets can be synthesized by soft-chemical exfoliation reaction and used as efficient building blocks for heterostructured nanohybrids, porous nanocomposites, multilayered films, freestanding hybrid films, etc. The resulting 3D hybrid materials possess diverse promising applicabilities for energy and environmental technologies. In this talk, several practical examples of the 2D inorganic/graphene nanosheets will be presented together with their self-assembled nanohybrids having tailorable physicochemical properties and functionalities such as electrode activity, photocatalytic activity, redox catalytic activity, electrocatalytic activity, gas adsorption capability, and nanobio application.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT1-4**

Area: Synthesis and Application of Two-Dimensional Materials

Type: Symposium, Time: FRI 10:25, Chair: Hyeon Suk Shin

Recent Progress in Large-Area Graphene Synthesis and Its Application to Advanced Chemical and Biological Analysis

Byung Hee Hong

Division of Chemistry, Seoul National University, Korea

Graphene has unique mechanical, electronic, and optical properties, which researchers have used to develop novel electronic materials including transparent conductors^{1,2} and ultrafast transistors, etc. Recently, understanding various chemical and optoelectronic properties of graphene has facilitated its application to high-performance devices that generate or store energy. Graphene is now expanding its territory beyond display/energy applications and moves toward biomedical research areas.³ In this talk, recent advances in the industrial production of CVD graphene films will be reviewed first, and novel chemical phenomena in 2-dimension enabled by the unique properties of graphene will be discussed, including graphene catalyzed/inhibited reactions,⁴ in-situ observation of 2D liquids in graphene liquid cell,⁵ unusual stability of biological samples under graphene layers,⁶ and novel optical/chemical behaviors of molecules between graphene layers.

References:

- [1] Kim, K. S. et al. Large-Scale Pattern Growth of Graphene Films for Stretchable Transparent Electrodes. *Nature* 2009, 457, 706 (2009)
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- [4] Shin, D., et al. Graphene oxide catalyzed cis-trans isomerization of azobenzene. *APL Mat.* 2014, 2, 092501.
- [5] Shin, D., et al. Growth Dynamics and Gas Transport Mechanism of Nanobubbles in Graphene Liquid Cells. *Nature Commun.* 2015, 6, 6068.

[6] Park, J. B. et al. Non-destructive electron microscopy imaging and analysis of biological samples with graphene coating. 2D Mater, 2016, 3, 045004.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: MAT2-1

Area: Current Trends in Energy Nanomaterials

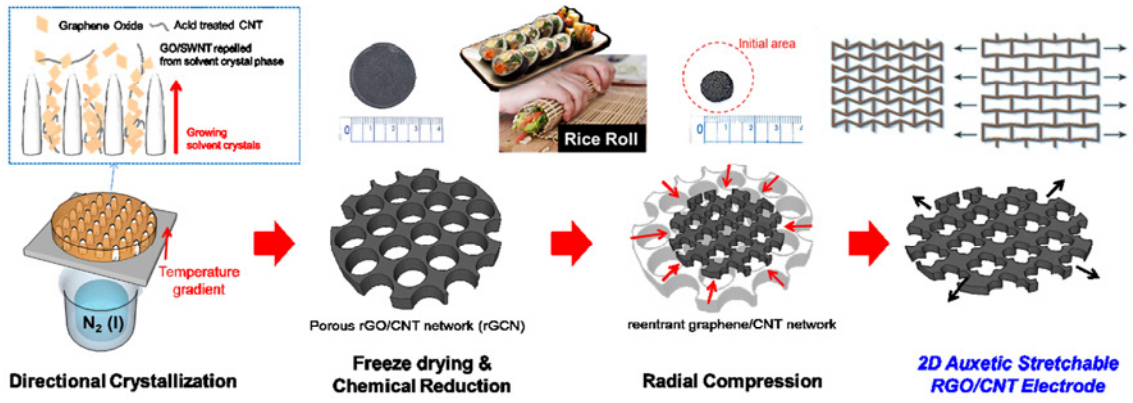
Type: Symposium, Time: FRI 14:30, Chair: Hye Ryung Byon

Nanostructured Graphene for Supercapacitor Electrodes with High Performance and Stretchability

Jeong Gon Son

Photo-electronic Hybrids Research Center, Korea Institute of Science and Technology, Korea

Chemically derived graphene oxide (GO) and its derivatives are promising candidates for a variety of carbon-based functional nanostructures and hybrid architectures, because of their unique characteristics that include high theoretical surface area, tunable electrical conductivity, excellent solution processability, and high mass producibility at low cost. However, the irreversible stacking due to the strong π - π interactions between graphene nanosheets during drying or reduction processes significantly decreases the solution processability as well as accessible surface area. In this talk, we fabricated three-dimensional (3D) graphene structures with templated-assisted crumpled graphene approach and directionally porous ice-templated approach for the energy storage application, such as supercapacitor electrodes. We introduce a sea urchin-like spiky template with simultaneous chemical etching/reduction process for the fabrication of 3D crumpled graphene balls. And, using a facile ice-templated self-assembly process with reduced graphene sheets and vanadium phosphate (VOPO₄) nanosheets, we realize a three-dimensional (3D) porous graphene/VOPO₄ nanosheet nanocomposite with high surface area and high electrical conductivity for the enhanced pseudocapacitive properties. In the last part, we also used the ice-templated vertically porous graphene nanostructures as a stretchable supercapacitor electrode. Radially compressed honeycomb structures exhibited nearly-zero poisson ratio structures and maintained their structure and electrical conductivity even at 50 % of stretched states. The capacitive performance of these compressed honeycomb structures also shows fairly high over 130 F/g and these high performance still be maintained at highly stretched condition.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT2-2**

Area: Current Trends in Energy Nanomaterials

Type: Symposium, Time: FRI 14:50, Chair: Hye Ryung Byon

Tin-based Alloy Anode Materials for Magnesium-ion Batteries

Seung-Wan Song

Dept. of Chem. Eng. & App. Chem., Chungnam National University, Korea

Rechargeable magnesium batteries have received a considerable attention as one of the beyond-lithium batteries for next-generation energy storage systems. The benefits of magnesium compared to lithium are earth abundance, low cost and higher theoretical volumetric capacity. The utilization of magnesium metal anode is often limited due to the irreversible formation of inactive surface blocking layer in conventional electrolytes and the limited choice of counterpart cathode material. Insertion-type materials such as tin, etc., which are based on the alloy reaction with magnesium, have recently been introduced as a new class of alternative anode materials to magnesium metal. Obtaining a good charge-discharge cycling performance of those new materials is however a huge challenge. We have been pursuing the development of tin-based alloy anode materials for the realization of magnesium-ion batteries. In this talk, we report our recent research results of the electrochemical performance and interfacial phenomena of tin-based anode materials. // This work was supported by National Research Foundation of Korea (2015062107).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT2-3**

Area: Current Trends in Energy Nanomaterials

Type: Symposium, Time: FRI 15:10, Chair: Hye Ryung Byon

Secondary Transformation of Nanocrystals for Electrochemical Energy Applications

Don-Hyung Ha

School of Integrative Engineering, Chung-Ang University, Korea

Secondary chemical transformations of as-synthesized nanocrystals (NCs) are an emerging and powerful method to tailor the composition and morphology of NCs. Nanosynthetic chemistry has centered on creating new NCs using these transformations. However, beyond works employing empirical qualitative analysis, few works have addressed the underlying atomic mechanisms for these transformations. Works using secondary chemical transformations of NCs for applications are also an under-studied field. This presentation spans from fundamental understandings of the atomic structural evolutions and mechanisms in chemical transformations for NCs, to use of these methods to create and characterize new structures, to the final applied stage of electrochemical energy applications of these chemically transformed materials, such as additive free battery electrodes and electrocatalysts for hydrogen evolution.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT2-4**

Area: Current Trends in Energy Nanomaterials

Type: Symposium, Time: FRI 15:30, Chair: Hye Ryung Byon

Domain- and template-engineered oxide epitaxial thin films as photoanodes for solar water splitting

Sanghan Lee

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

Recently, complex oxides epitaxial thin films have gained much attention due to their novel properties as a photoelectrode for hydrogen production via solar water splitting. We present two fundamental studies about BiFeO₃ and BiVO₄ which are well known as a promising photoanode. First topic is about domain-engineered BiFeO₃. BiFeO₃ has different spontaneous polarizations and ferroelectric domain structure depending on the crystallographic orientations, so it is of great significance to clarify the direct relationship between photocatalytic properties, spontaneous polarizations and ferroelectric domain structures. Considering the above, we revealed the most enhanced photocatalytic performances of BiFeO₃ could be shown in the (111)_{pc} BiFeO₃, due to its high spontaneous polarization and mono-variant domain structure. Furthermore, ferroelectric polarization switching in the (111)_{pc} BiFeO₃ caused an approximate change of 8,000% in the photocurrent density. Second topic is about template-engineered BiVO₄ epitaxial thin films. It is necessary to demonstrate high quality epitaxial films to explore their fundamental properties. In this study, the growth of epitaxial BiVO₄ is investigated using a thin γ -WO₃ template layer. Consequently, the photocurrent density of epitaxial BiVO₄ on the γ -WO₃ template layer is approximately 10 times greater than that of bare BiVO₄, related to the effective charge transfer by the γ -WO₃ intermediate layers.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT2-5**

Area: Current Trends in Energy Nanomaterials

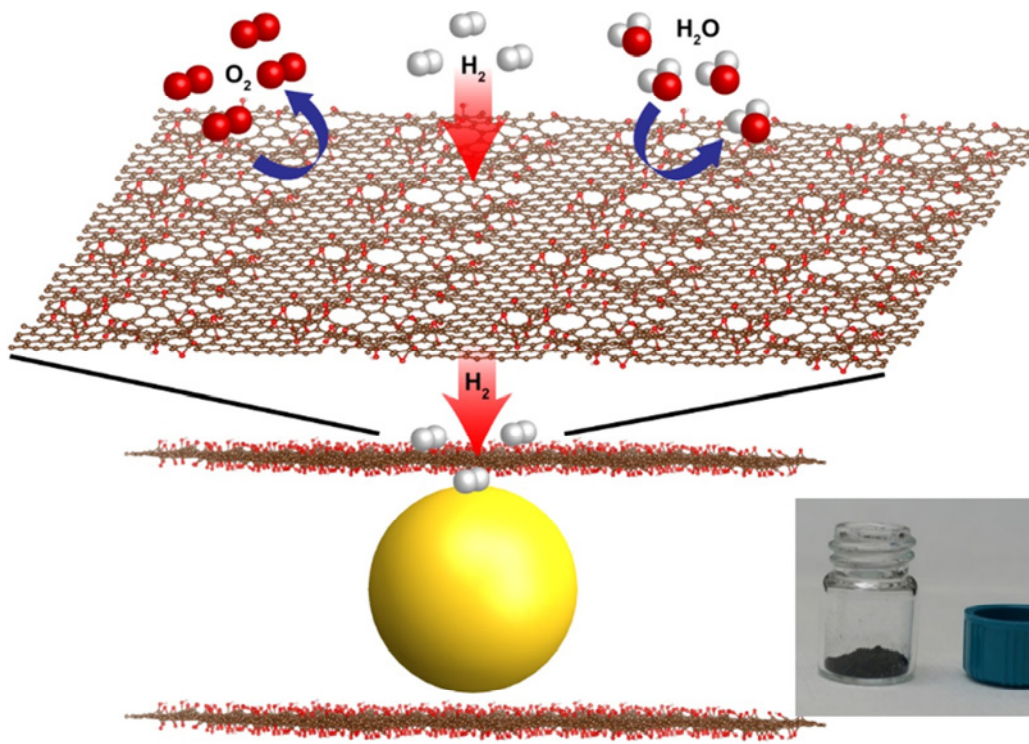
Type: Symposium, Time: FRI 15:50, Chair: Hye Ryung Byon

Fueling the Future: High-Density Hydrogen Storage in Hybrid Nanomaterials

Eun Seon Cho

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

Graphene and its derivatives offer a variety of opportunities for applications in gas transport and separation. It is mainly attributed to their atomically thin and mechanically excellent properties. Particularly, it was reported that hydrogen is allowed to be penetrated through graphene oxide layers, while other large gas molecules such as oxygen are not. Hydrogen has been considered as an ultimate clean energy source without emitting greenhouse gases. To realize hydrogen economy, it is of paramount importance to develop a high-performance hydrogen storage material—achieving a high storage capacity with enhanced kinetics under reasonable operating temperature and pressure—simultaneously mitigating hydrogen-related safety concerns. In this talk, a new multilaminate comprised of magnesium nanocrystals and reduced graphene oxide layers will be explored for safe and efficient hydrogen storage. Combining a hydrogen-selective characteristic of graphene oxide layers with an excellent storage capability of magnesium, a high-performance hydrogen storage material was successfully exploited, also presenting a remarkable air-stability.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC1-1**

Area: Current Trends in Electrochemistry for Energy Conversion

Type: Symposium, Time: THU 13:30, Chair: KI MIN NAM

Design of New Materials for Next-Generation Solar Cells

Hyosung Choi

Department of Chemistry, Hanyang University, Korea

Development of new photovoltaic materials (transparent conducting electrodes, light harvesting semiconductors, and charge transport materials) has been required for high-performance next-generation solar cells including polymer and perovskite solar cells. Here, we introduce silver nanowire (Ag NWs)-based electrodes prepared via various methods and patternable PEDOT:PSS conducting polymer electrode by cross-linking agent. Because of simple processing technique, high transmittance of over 85% in visible wavelength region and high electrical conductivity over 1000 S/cm, those electrode materials can be used as transparent electrode for optoelectronic devices including solar cells and light-emitting diodes instead of conventional ITO electrode.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC1-2

Area: Current Trends in Electrochemistry for Energy Conversion

Type: Symposium, Time: THU 13:55, Chair: KI MIN NAM

High efficiency oxygen evolution from water using elaborately designed hematite photoanodes

Hyunwoong Park

School of Energy Engineering, Kyungpook National University, Korea

Molecular hydrogen (H₂) produced via solar water splitting has received growing attention as a renewable and carbon-neutral energy carrier over the past four decades. To drive high-efficiency solar H₂ production, significant effort has been focused on photoelectrochemical (PEC) water oxidation, particularly in terms of reducing overpotential while increasing photocurrents for the oxygen evolution reaction (OER) at $E = 1.23$ V. Among the many semiconductor photoanode materials reported in the literature, hematite (α -Fe₂O₃) is considered the most suitable. However, hematite suffers from poor solar-to-hydrogen (STH) efficiency (i.e., small photocurrent densities at 1.23 V) and rapid deactivation, primarily because of its short hole-diffusion length (2-4 nm), rapid charge recombination, sluggish charge transfer, and inefficient charge injection. These challenges have been traditionally addressed by adopting problem-specific strategies including doping, passivation, and coupling with OER catalysts. Nevertheless, the PEC performance of hematite is still poor in terms of photocurrent and durability. Herein, we report the synthesis of ultra-highly efficient and durable hematite nanorod arrays developed by elaborate engineering and careful optimization of three surface modification methods, i.e., hydrogen treatment, coating with a TiO₂ passivation layer, and deposition of cobalt phosphate OER catalyst. Each modification significantly affected the PEC performance, while integration of all three modifications led to unprecedented photocurrents of ~ 6 mA/cm² at 1.23 V over 100 h under simulated sunlight (AM 1.5G, 100 mW/cm²). The Faradaic efficiency of O₂ evolution was over 95%, and a stoichiometric amount of H₂ was simultaneously produced.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC1-3**

Area: Current Trends in Electrochemistry for Energy Conversion

Type: Symposium, Time: THU 14:20, Chair: KI MIN NAM

Gold Nanoclusters: A New Light Harvesting Antenna for Solar Energy Conversion

Jin Ho Bang

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

Gold nanoclusters (Au NCs) with molecule-like behavior have emerged as a new light harvester in solar energy conversion systems. Despite several important strides made recently, efforts toward the utilization of NCs as a light harvester have been primarily restricted to proving their potency and feasibility. A complete characterization of metal cluster-sensitized solar cells (MCSSCs) is still lacking, and hence comprehensive understanding of the interfacial events and limiting factors that dictate their performance remains elusive. In this presentation, the investigation on the effect of the size of the Au NCs and electrolytes on the performance of MCSSCs is presented and their implication in MCSSCs is discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ELEC1-4

Area: Current Trends in Electrochemistry for Energy Conversion

Type: Symposium, Time: THU 14:45, Chair: KI MIN NAM

Hydrogen Evolution Reaction using Layered Ternary Transition Metal Chalcogenide and Blue TiO₂ Nanomaterials

Anand prakash Tiwari, Hyoyoung Lee^{1,*}

Material science and engineering, Korea Advanced Institute of Science and Technology, Korea

¹*CINAP-IBS, Department of Chemistry, Korea*

Layered ternary transition metal chalcogenides (TTMCs) material has been paid attention to overcome to the limitation of active sites which is challenging in binary transition metal chalcogenides (BTMC), such as MoS₂, towards electrochemical hydrogen production. Here, we demonstrate TTMC material which contains two transition metals Cu and Mo with chalcogen S. The TTMC, Cu₂MoS₄ has been successfully synthesized by a facile solution-processed method. Moreover, by anion doping such as Se in as the synthesized Cu₂MoS₄, it has been found that TTMC can be exfoliated into single layer nanosheets. Furthermore, by controlling the number of layers, single layers TTMC exhibit the highest electrocatalytic activity towards hydrogen evolution reaction (HER) because the single layers can provide more catalytic active sites than multilayers and bulk. As a result, our TTMC work can guide new strategy for the developments of applications of TMCs in HER. In addition, we like to also introduce new visible-light driven blue TiO₂ materials for photo-catalytic HER.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC1-5**

Area: Current Trends in Electrochemistry for Energy Conversion

Type: Symposium, Time: THU 15:10, Chair: KI MIN NAM

Strategies for the development of dichalcogenide anode materials for advanced Na ion storage

Yong-Mook Kang

Department of Energy and Materials Engineering, Dongguk University, Korea

Considering that the high capacity, long-term cycle life, and high-rate capability of anode materials for sodium-ion batteries (SIBs) is a bottleneck currently, a series of Co-doped FeS₂ solid solutions with different Co contents were prepared by a facile solvothermal method, and for the first time their Na storage properties were investigated. The optimized Co_{0.5}Fe_{0.5}S₂(Fe_{0.5}) has discharge capacities of 0.220 Ah/g@1 after 5000 cycles at 2 Ag@1 and 0.172 Ah/g@1 even at 20 Ag@1 with compatible ether-based electrolyte in a voltage window of 0.8–2.9 V. The Fe_{0.5} sample transforms to layered Na_xCo_{0.5}Fe_{0.5}S₂ by initial activation, and the layered structure is maintained during following cycles. The redox reactions of Na_xCo_{0.5}Fe_{0.5}S₂ are dominated by pseudocapacitive behavior, leading to fast Na⁺ insertion/extraction and durable cycle life. A Na₃V₂(PO₄)₃/Fe_{0.5} full cell was assembled, delivering an initial capacity of 0.340 Ah/g@1.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC2-3

Area: Recent Advances in Electrochemistry

Type: Award Lecture in Division, Time: FRI 10:20, Chair: Jun Hui Park

Use of Nanoscale Functional Materials in Electrochemiluminescence: Making Electrochemiluminescence Brighter

Joohoon Kim

Department of Chemistry, Kyung Hee University, Korea

Electrochemiluminescence (ECL) is a unique luminescent phenomenon in which electrochemically generated species are involved to form excited states emitting light. Since ECL provides beneficial characteristics over photoluminescence, including low background emission, good temporal and spatial controllability, robustness, and instrumental simplicity, the ECL technique has been utilized as a versatile tool in a variety of electroanalytical applications. Especially, since Bard and his co-workers presented for the first time a new approach for generating ECL (*i.e.*, coreactant pathways) in the 1980s, the ECL technique has been achievable in aqueous environment, and thus been popular to the clinical and bioanalytical applications. To further expand the usefulness of ECL in the applications, many promising approaches have been suggested for amplification of ECL signals. Of the approaches, we recently reported the use of nanoscale functional materials such as dendrimer-encapsulated nanoparticles and chemically converted graphenes for the enhancement of ECL. In the present talk, as a humble first-step to the long journey toward making ECL brighter, we discuss mainly about the use of dendrimers for enhanced ECL. First, we discuss highly enhanced ECL of $\text{Ru}(\text{bpy})_3^{2+}$ (bpy = 2,2'-bipyridyl) or luminol with appropriate coreactants on electrodes modified with amine-terminated dendrimers encapsulating catalytic nanoparticles. Second, we discuss intense ECL of $\text{Ru}(\text{bpy})_3^{2+}$ in the presence of amine-terminated dendrimers as a coreactant especially when utilizing intramolecular reactions between $\text{Ru}(\text{bpy})_3^{2+}$ and dendrimers.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC2-1

Area: Recent Advances in Electrochemistry

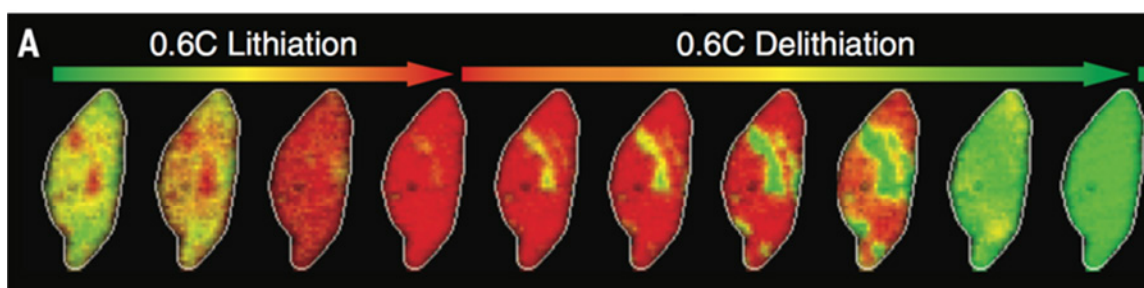
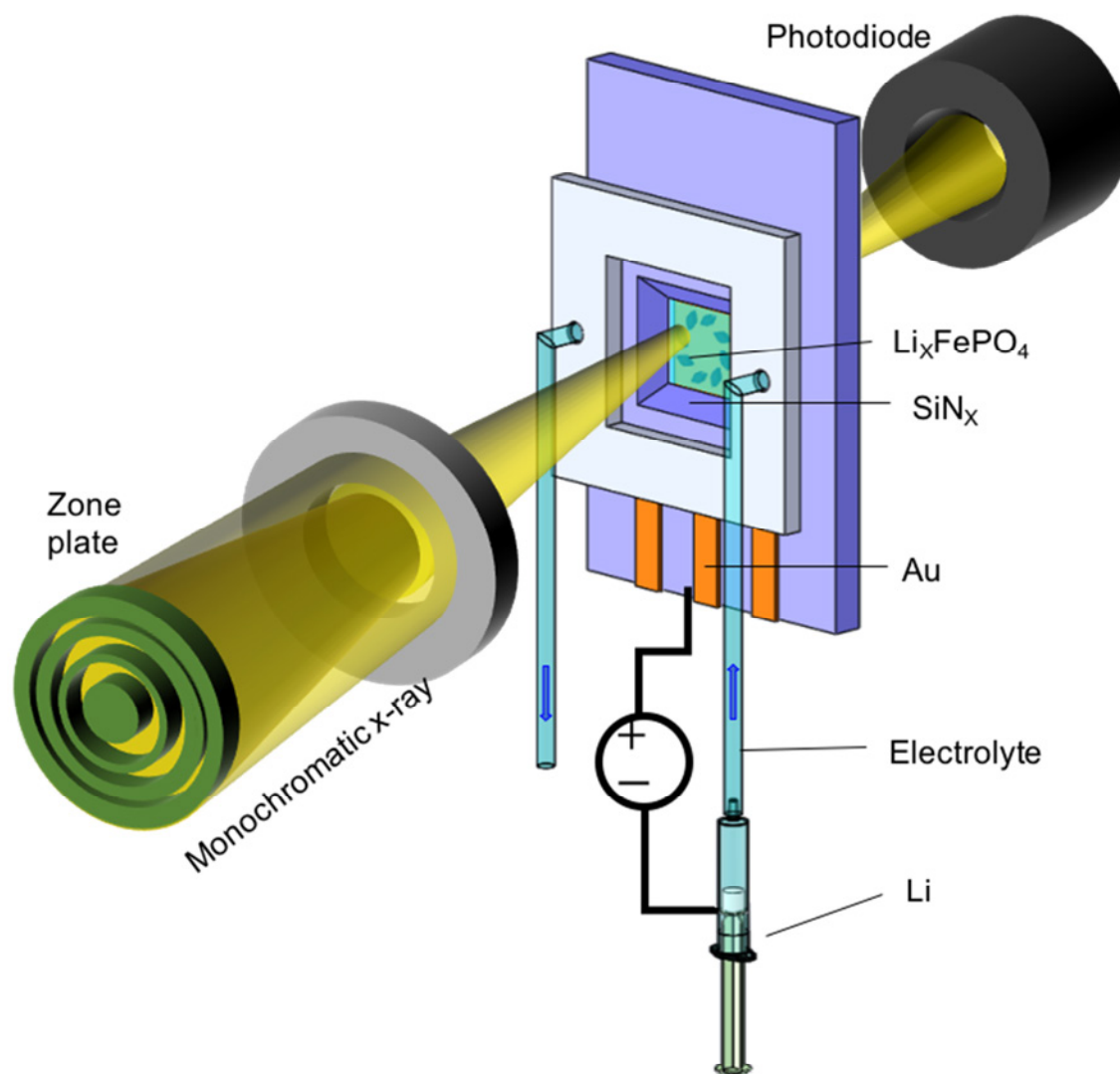
Type: Symposium, Time: FRI 09:10, Chair: Jun Hui Park

Bringing single-level spectromicroscopy to electrochemical systems : lithium ion batteries and microbial fuel cells

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

Electrochemistry plays a significant role in energy conversion and storage technologies, such as lithium ion batteries (LIBs) and microbial fuel cells (MFCs). Specifically, LIBs are constructed using billions of individual battery particles, which store (or generate) the electrical energy by forming (or breaking) the chemical bonds with lithium ions within the particle. MFCs are also the electrochemical devices consisting of the bio-electrodes where billions of microorganisms convert high-energy chemical bonds to electrical energy. For these applications, the electrochemical kinetics or thermodynamics of the individual bacterium or battery primary particle defines the fundamental limit of the devices, and further governs the overall performance. However, due to the porous and heterogeneous nature of these electrodes, the conventional current-voltage measurement on these ensembles shows the certain limit in untangling complexity and heterogeneity of electrochemistry. Here, in my talk, I will introduce the electrochemical platform where synchrotron-based spectromicroscopy (or optical microscopy) and electrochemical microfluidic cells are combined to investigate the charge transfer mechanism at a single bacterium or a single primary battery particle. The detailed spatiodynamics within battery particles gained from this platform will be highlighted.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC2-2

Area: Recent Advances in Electrochemistry

Type: Symposium, Time: FRI 09:40, Chair: Jun Hui Park

Noble Metal-Based Bimodal Nanocatalysts for Hydrogen Evolution Reaction in an Alkaline Electrolyte

Sang-II Choi

Department of Chemistry, Kyungpook National University, Korea

Hydrogen evolution reaction (HER) in an alkaline media consumes massive electrical energy during water electrolysis owing to the sluggish kinetics. Therefore, development of an active electrocatalyst is remained as the great challenge. Because the Pt catalyst showing the best activity among the HER catalysts, is expensive, development of the cost-effective electrocatalyst has been intensively studied by many researchers. Recent reports designed the bimodal surface modified catalysts, such as noble metal-transition metal hydroxides composites, as the promising candidate for enhancing the alkaline HER kinetics. In this bimodal system, the oxophilic metal hydroxides catalyze the dissociation of water and the formation of hydrogen intermediates, while the nearby noble metal surface converts the hydrogen intermediate to H₂ gas. In this talk, we introduce the effective electrocatalysts based on Ru nanocrystals, where Ni(OH)₂ was formed on their surfaces during a synthesis. The as-prepared bimodal electrocatalysts show comparable HER activity with that of a commercial Pt/C catalyst.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU1-1**

Area: Current Trends in Chemistry Education

Type: Symposium, Time: FRI 09:00, Chair: Sukjin Kang

Science Fiction in Science Education

HyunJu Park

Chemistry Education, Chosun University, Korea

Imagination is a base of tool of creativity. When a scientific imagination combines with an artistic imagination, a 'wonderful imagination' is completed. Science Fiction (SF) is a completion of representative 'great imagination'. Science fiction is a science fiction novel, which is a science fiction genre based on scientific knowledge. The advantages of using science fiction in science education are summarized as follows. First, science fiction is a great tool to stimulate students' intellectual curiosity and creative imagination to begin scientific inquiry. Second, science fiction guides students to find the scientific principles, misconcepts, and the metaphysical issues (eg, human consciousness, individual identity, origin of the universe, the nature of space and time) underlying novel. Third, science fiction provides an opportunity to recognize the relationship between science, culture, and society. Fourth, science lessons are a great way for students to develop imagination between science and language or art. This kind of science fiction is a useful tool for students in humanities and plays a key role in science education. However, in Korea, science education using science fiction is still a rudimentary stage in practical field application or research. Therefore, in this study, it is aimed to investigate a possibility of a new approach using science fiction in Korean science education.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: EDU1-2

Area: Current Trends in Chemistry Education

Type: Symposium, Time: FRI 09:30, Chair: Sukjin Kang

Overseas Voluntary Activities and Science Education

JaeYoung Han^{*}, Sungmin Im¹

Department of Chemistry Education, Chungbuk National University, Korea

¹Faculty of Science Education, Daegu University, Korea

Recently in Korea many science teachers have participated in overseas voluntary activities. Korea is the only nation that has changed into a donor country from a recipient country in the international aid. Many senior science educators could have seen the equipments of science experiment in the school laboratory that had come by the IBRD loan. Without doubt, the science education was one of the basic foundation of the development of Korea. I participated several overseas voluntary activities, and analyzed the activities with cultural historical activity theory (CHAT). The CHAT is the tool of analyzing any human activity system into six elements to find the structure of the activity and the conflicts in the activity. The six elements are subject, object, tools, community, rule, and division of labor. I compared the activity by in-service science teachers with the one by pre-service teachers. In doing so, I searched the implication of overseas voluntary activity on the science education. The science teachers could reconfirm the goal of science education as a basis of national development. Also the teachers could rethink the role of science experiment, as a tool of cognitive understanding or a method of motivation of science learning. The pre-service teachers could have a good chance of practicum where they can learn many things related to science teaching and learning. Overall, the overseas voluntary activities give science teachers the chance of reflection on their life as a science educator. (This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2015S1A5A2A03048047))

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU1-3**

Area: Current Trends in Chemistry Education

Type: Symposium, Time: FRI 10:20, Chair: Sukjin Kang

Creative convergence science lab: Design and implementation

Jeongho Cha

Faculty of Science Education, Daegu University, Korea

Creative Convergence Science Lab (CCSL), which is based on the master plan of science education during 2016-2020, is a project for enforcing future science learning environment through innovating old science laboratory into high-tech science lab in which students can do STEAM related inquiry activities with digital inquiry tools. In 2016, a design of conceptual model for CCSL and teaching and learning model for CCSL were developed. As a result of field study and conceptual design, the project team divided spaces of science lab into several modules such as coaching/presentation module, learning module, experiment/inquiry module, team-based cooperation module, container/preparation (data-point) module, and moving module, which can be combined flexibly according to the context and the need that every school are facing. Various types of instructions which can be done in CCSL were also developed and suggested. These instructions are curriculum based instruction, high-tech (IoT, wearable machine, digital technology, etc.) based instruction, and open source data/big-data based instruction. In 2017, 50 model schools including primary and secondary schools were selected and the models developed is being applied. In this talk, the design and implementation process of CCSL will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU2-1**

Area: Chemistry Education for the Science Gifted Students

Type: Symposium, Time: FRI 14:30, Chair: JaeYoung Han

KSA Experience-Based Learning Programs

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

Science gifted students are curious in their field of interest and show high concentration. In order for students with science talent to grow to become excellent scientists of the future, the growth as future scientists, above all, confidence in their appearance is necessary. Science talented students will develop confidence in their own appearance while talking with scientists as well as experiences of scientific experiments in high school. Not only the program of research activities but also the outsourcing education program and the international collaborative research program make it possible for students to have such confidence not only the scientific experience that they can grow into excellent future scientists. In this study, I think that students at Korean Science and Gifted School have a great foundation for growth as scientists through the curriculum research activity program, especially R & E research activities. Also, I would like to share my experiences of growing chemistry through outsourcing education program and international collaborative research program.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU2-2**

Area: Chemistry Education for the Science Gifted Students

Type: Symposium, Time: FRI 14:50, Chair: JaeYoung Han

Research & Education Program in Science High School for the Gifted

Mi Young Han

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

This symposium of chemistry education for the science gifted students is rooted in Chemistry Education Forum for chemistry teachers in six science high schools for the gifted. The Chemistry Education Forum provided the place where chemistry teachers in science high school for the gifted shared the information and experiences on curriculum, R&E programs and new teaching strategies for the gifted students. Practical discussions on running the education programs like informal activities, research programs and education contents were actively made. In this context, this report is intended to show the practical cases of running R&E programs in Daejeon Science High School for the Gifted and suggest the need for finding a new approach to R&E programs in science high school for the gifted. Many studies for the R&E program were published to evaluate the effect and running status of R&E programs in science high school based on statistical studies or qualitative surveys. But unlike previous studies, this report is based on experience in mentoring the R&E programs as a science high school teacher and intended to initiate the discussion on the running R&E programs supplying with actual R&E mentoring cases.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU2-3**

Area: Chemistry Education for the Science Gifted Students

Type: Symposium, Time: FRI 15:10, Chair: JaeYoung Han

Educational significance of R & E activities in university

Chang-Hoon Nam

Daegu Gyeongbuk Institute of Science & Technology, Korea

R & E activities centring on science gifted and talented young scientists are taking place within the university. The main theme of R & E activities is mainly based on experimental subjects of research labs in university, and activities are being carried out with the help of graduate students and researchers. These activities have the meaning of experiencing the experimental process which is difficult to experience in the high school course in advance. I think it is important to plan the desirable R & E activities to look at the educational significance of these preliminary activities. I would like to take a step further and look at what R & E programs can better cultivate the active competence and creativity of R & E participating students. We will discuss the limitations of R & E activities that are currently being undertaken at existing universities, as well as the future direction while looking at the above themes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR-1

Area: R&D beyond Carbon Society I

Type: Award Lecture in Division, Time: THU 13:30, Chair: Jaeyoung Lee

Unique chemical processes in ice and its environmental impacts

Kitae Kim

Korea Polar Research Institute, Korea

In general, most chemical reactions are slowed down when temperature drops according to the Arrhenius equation. However, specific chemical processes are accelerated in ice phase. Takenaka et. al., found that the oxidation of NO₂⁻ to NO₃⁻ in the presence of oxygen was significantly enhanced by freezing.(105 times accelerated compared to the aqueous solution) Although the chemical processes in frozen state play a significant role on various Earth's system, they have rarely been studied. The environmental fate, bioavailability, mobility, and toxicity of metals or inorganic elements are controlled by their redox speciation. In this talk, I want to introduce our previous results(1. enhanced chemical dissolution of metal oxide particles in ice, 2. accelerated chemical transformation and toxicity decrease of harmful heavy metals in ice, 3.enhanced oxidation of iodide to reactive iodine species in ice and release to the gas phase) and future research topics about unique chemical transformation processes in ice phase.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR-2

Area: R&D beyond Carbon Society I

Type: Symposium, Time: THU 14:10, Chair: Jaeyoung Lee

Electrochemistry at an interface between two immiscible electrolyte solutions for Energy and Environmental Applications

Hye Jin Lee

Department of Chemistry, Kyungpook National University, Korea

Over the last two decades, charge transfer reactions at an interface between two immiscible electrolyte solutions (ITIES) have attracted great attentions in research fields of analytical, pharmaceutical, biological and energy related applications. In this talk, we will highlight our recent efforts made on investigating voltammetric characterization of charge transfer processes at a polarized ITIES (e.g., water/1,2-dichloroethane, water/polyvinylchloride-nitrophenyloctyl ether) for carbon dioxide reduction to produce formate and hydrogen gas in addition to developing ion selective and sensitive sensing platforms for formate fuel and some of water pollutants. Various electrochemical techniques including cyclic, linear sweep, and differential pulse voltammetries alongside chronoamperometry were employed to monitor the charge transfer process across the ITIES. Some of interesting preliminary results and future aspects of ITIES will also be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR-3

Area: R&D beyond Carbon Society I

Type: Symposium, Time: THU 14:50, Chair: Jaeyoung Lee

Oxidation of CO, toluene and acetaldehyde catalyzed by mesoporous- template-supported NiO and Fe₂O₃ nanoparticles prepared by vapor deposition methods

Young Dok Kim

Department of Chemistry, Sungkyunkwan University, Korea

Atomic layer deposition (ALD) is a widely used technique in the semiconductor industry for the fabrication of ultrathin films. Recently, application of this technique has been extended to the incorporation of catalytically active nanoparticles within mesoporous structures. On the other hand, temperature-regulated chemical vapor deposition (TR-CVD) has been recently shown to be as effective as ALD for insertion of nanoparticles into the mesoporous templates. In this talk, recent progress in synthesis of nanocatalysts based on ALD and TR-CVD will be shortly reviewed. NiO or Fe₂O₃ nanoparticles could be incorporated into mesoporous SiO₂ and Al₂O₃ substrates and not only the surface topmost part of the substrate particles but also deeper layers with a depth of several tens to hundreds of micrometer could be decorated by NiO or Fe₂O₃ nanoparticles. The catalysts prepared in this way were shown to be highly active for low temperature CO, acetaldehyde and toluene oxidation. Particularly, unique structure of our catalysts consisting of nanoparticles confined within mesopores showed high stability of catalytic activity as well as resistance to poisoning by SO₂. X-ray Photoelectron Spectroscopy was used to shed light on the structure of active sites of each catalyst for various reactions, which will be reviewed in this talk.

Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: ENVR-4

Area: R&D beyond Carbon Society I

Type: Symposium, Time: THU 15:20, Chair: Jaeyoung Lee

Suggestion on the Energy Industry from Atmospheric Environmental Perspective for Air Quality Improvement

Kyung-Eun Min

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

Due to continuous industrial and economic developments, humanity in the world is living a life that requires more energy than ever before. As a result, the environmental burden associated with energy production is also increasing. In particular, the degree of atmospheric environmental load in these days specifically in northeast Asia has been so serious that it affects the daily life of the general public beyond academical interest. High concentrations of ultrafine particles and ozone are the major examples of atmospheric issues we are facing in these day. In this presentation, we will discuss the connection between the energy industry and contemporary air pollution issue through the latest academic knowledge from atmospheric view.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS1-1**

Area: [Tutorial] NMR Applications in Chemistry

Type: Symposium, Time: WED 15:00, Chair: YONGAE KIM

Structure Determination of Small Organic Compounds by Solution NMR Method

Jung-Rae Rho

Kunsan National University, Korea

Solution Nuclear Magnetic Resonance (NMR) is an excellent tool for determining the structures of small organic compounds like natural products at the level of individual atoms. Instead of a direct picture or image of the molecule, the structure can be interpreted by a series of NMR spectra which provide the connectivity between an atom and its neighboring atoms in the molecule. In many cases 1D NMR (^1H and ^{13}C) and 2D NMR (COSY, TOCSY, HSQC, and HMBC) experiments routinely enabled us to determine the planar structure of a molecule less than 1000 Da and also NOESY/ROESY experiment established the relative configurations within the rigid part of the molecule. In this presentation, the nature of these experiments will be dealt in more detail, and all these experiments will be applied to determine the structure of a natural product as an example.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS1-2**

Area: [Tutorial] NMR Applications in Chemistry

Type: Symposium, Time: WED 16:00, Chair: Jung-Rae Rho

Introduction of SOLID-STATE NMR Spectroscopy for Chemicals and Polymer Materials

YONGAE KIM

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Conventional analytical methods like XRD and IR spectroscopy have lots of limitations to study the structure, conformation and morphology for solid-state powdered samples. Therefore, demands for the solid-state NMR spectroscopy become larger and larger for a variety of solid-state samples. Here, we will discuss about the basic theory and solid-state NMR characterization of nano- and bio- materials like polymers, inorganic materials, battery related materials, pharmaceutical drugs, antimicrobial peptides, disease related membrane proteins etc. And home-built solid-state NMR probe for in-situ measurements also will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS2-1**

Area: Scientific and Technological Talents Aspired by the Government and Industry

Type: Symposium, Time: THU 10:00, Chair: Youngeun Kwon

The Role of Chemists at the heart of the Fourth Industrial Revolution

Inho RHA

Vice-president of DONGWOO FINE-CHEM, Korea

1. Company Overview: DONGWOO FINE-CHEM

2. What is the desirable role of chemists in the era of the Fourth Industrial Revolution?

Google's Computer Program, AlphaGo, defeated Lee Sedol, a South Korean master of Go in the Google DeepMind Challenge Match in March 2016, winning the five game match with a 4-1 score. Since its historic success, AlphaGo has heralded a new era for the ancient game of Go with worldwide interest as to whether machines could overcome the creativity and thinking skills considered as unique human domains. Thereafter, interest in artificial intelligence and the new paradigm of the Fourth Industrial Revolution increased dramatically.

Slightly ahead of this turn of century match, "Mastering the Fourth Industrial Revolution" was set as a major agenda item at the World Economic Forum (WEF) held in Davos, Switzerland, in January 2016. The term 'the Fourth Industrial Revolution' itself was used to mean the convergence of manufacturing and information communication in 'High Tech Strategy 2020' announced by Germany in 2010. Since then, scientists, economists, and research institutes around the world have studied and discussed not only the Fourth Industrial Revolution but also the changes in future social structures and industrial forms that may arise.

Professor Klaus Schubert, author of the 4th Industrial Revolution and WEF Chair, defined the Fourth Industrial Revolution as a technological revolution that rapidly transforms economic and social structures through convergence of diverse sectors such as digital and biotechnology industries. On the other hand, it is also true that inconsistencies and confusion over the background, definition and features of the Fourth

Industrial Revolution are still growing. Since the Fourth Industrial Revolution has just begun, it can be interpreted differently depending on the interests of viewers, stakeholders, and countries.

In this presentation, I like to discuss about the desirable role of chemists in the Fourth Industrial Revolution era which will transform labor market resulting in a net loss of over 5 million jobs in 15 major developed and emerging economies by 2020.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: KCS3-1

Area: [IBS Symposium] Developing New Catalytic Organic Reactions and Investigating Their Applications

Type: Symposium, Time: WED 15:00, Chair: Sukwon Hong

Development of Direct C-H Amination Reactions

Sukbok Chang

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

Aryl amines are a key synthetic unit widely utilized in organic synthesis, coordination chemistry, materials science and pharmaceutical industry. Current routes to those compounds require either prefunctionalized starting materials or external oxidants, thus inevitably generating stoichiometric amounts of side wastes. We have developed a series of direct amidation and amination reactions of arene and alkene carbon-hydrogen (C-H) bonds using organic azides as the amino source releasing molecular nitrogen as the single by-product. More recently, 1,4,2-dioxazol-5-one and its derivatives have also been proved as the highly efficient and robust amino sources in this direct C-H amination. The reaction is catalyzed by a cationic rhodium, iridium, or cobalt complex under external oxidant-free conditions, and a broad range of chelate group-containing arenes are selectively amidated and aminated with excellent functional group tolerance, thereby opening a new avenue to environmentally benign carbon-nitrogen (C-N) bond formation which can be immediately applied in synthetic chemistry, medicinal, and materials science.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: KCS3-2

Area: [IBS Symposium] Developing New Catalytic Organic Reactions and Investigating Their Applications

Type: Symposium, Time: WED 15:20, Chair: Sukwon Hong

Decarboxylative C-H Activation for the synthesis of homoisoflavonoids & Decarboxylative trichlorination

Sunwoo Lee

Department of Chemistry, Chonnam National University, Korea

The development of simple and convenient method for the preparation of aryl alkynoic acids made it easy accessible tool for the introduction of alkynyl group in organic synthesis. In this presentation, we would like to discuss some of our recent research progress towards the decarboxylative coupling reactions of alkynoic acids. This presentation will cover the ruthenium-catalyzed decarboxylative C-H activation for the synthesis of homoisoflavonoids and metal-free decarboxylative trichlorination of alkynoic acid for the synthesis of trichloromethylketones. Homoisoflavonoid and flavone were selectively obtained from the reaction with salicylaldehydes and arylpropionic acid in the presence of ruthenium catalyst and base. When the reaction was conducted in DMSO, a variety of homoisoflavonoids were exclusively obtained in good yields. While, several flavones were dominantly formed under *t*-AmOH solvent. 2,2,2-Trichloroacetophenone derivatives were synthesized via decarboxylative trichlorination from arylpropionic acids and trichloroisocyanuric acid (TCCA). The reaction was conducted in the presence of H₂O at room temperature, and afforded the desired products in good yields. The reaction showed good functional group tolerance towards halides, cyano, nitro, ketone, ester and aldehyde groups. In addition, 2,2,2-trichloroacetophenone derivatives were readily transformed into esters, amides, and hydrazides.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: KCS3-3

Area: [IBS Symposium] Developing New Catalytic Organic Reactions and Investigating Their Applications

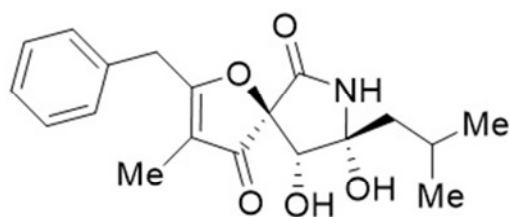
Type: Symposium, Time: WED 15:40, Chair: Sukwon Hong

Total Synthesis of Spirocyclic PKS-NRPS-Based Fungal Metabolites

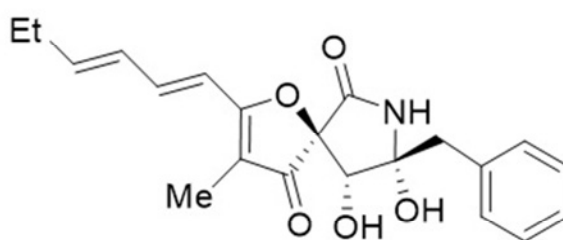
Sunkyu Han

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

Total synthesis of spirocyclic fungal metabolites (±)-berkeleyamide D and (±)-azaspirene will be presented. Structural analysis and reported biosynthetic studies of •hydroxy/methoxy-•lactam-based natural products prompted us to devise a biomimetic synthetic solution to these natural products. We constructed the key spirocyclic structure via a series of oxidations and cyclizations of biosynthetically relevant linear precursors. Notably, while our streamlined syntheses of berkeleyamide D and azaspirene sought inspiration from its biogenesis, our experimental data on chemical reactivity of biosynthetically relevant precursors conversely provide insights to the biosynthesis of natural products of this family



berkeleyamide D



azaspirene

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS3-4**

Area: [IBS Symposium] Developing New Catalytic Organic Reactions and Investigating Their Applications

Type: Symposium, Time: WED 16:20, Chair: Sunkyu Han

Development of Bifunctional N-Heterocyclic Carbene Ligands

Sukwon Hong

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

Cooperative catalysis enabling simultaneous activation of both an electrophile and a nucleophile has emerged as a powerful strategy in organic synthesis. We envision that imidazo[1,5-a]pyridine-derived N-heterocyclic carbene (ImPy) ligands will provide a convenient framework where a various functional group can be easily implemented to make bifunctional N-heterocyclic carbene ligands. Several transition metal complexes containing imidazopyridinylidene carbene (ImPy) ligands have been prepared. The ImPy-Cu(I) complexes efficiently catalyzed the direct C-H carboxylation of benzoxazole with CO₂. ImPy-Pd catalysts exhibited good reactivity in Buchwald-Hartwig amination reactions. Current progress on design of new bifunctional ImPy transition metal catalysts will be discussed in details in the presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS3-5**

Area: [IBS Symposium] Developing New Catalytic Organic Reactions and Investigating Their Applications

Type: Symposium, Time: WED 16:40, Chair: Sunkyu Han

Bidentate Directing Group: Versatile Platform for C–H Activation and Privileged Building Blocks

Sungwoo Hong

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

Solutions to problems that are posed by organic, medicinal, biological and material science, demand synthetic innovation with efficient synthetic routes. Our current research is focused on studying breakthrough knowledge in catalytic synthetic methods and molecular design that have high impact on broader scientific fields. The selective C–H bond functionalization has become the favored reaction methods in practical synthetic processes. The new catalytic synthetic methods allow us to perform the unprecedented disconnection of target molecules, affording innovative and imaginative synthetic strategies of so-called “privileged scaffolds”. The power and efficiency of direct C–H functionalization could be further enhanced by combining such catalytic transformations into a one-pot process, which is highly desirable by providing a powerful platform for constructing complicated key motifs from simple starting materials. Subsequent medicinal chemistry studies involving a modular approach and privileged fragments assembly, will provide bases for the development of pharmaceutical agents via structure-based design. The new catalytic synthetic methods will function as competent tools directly utilized in cross coupling reactions capable of connecting privileged building blocks, providing opportunities for the successful implementation of fragment-based drug design (FBDD) and eventually streamline drug discovery research.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-1**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

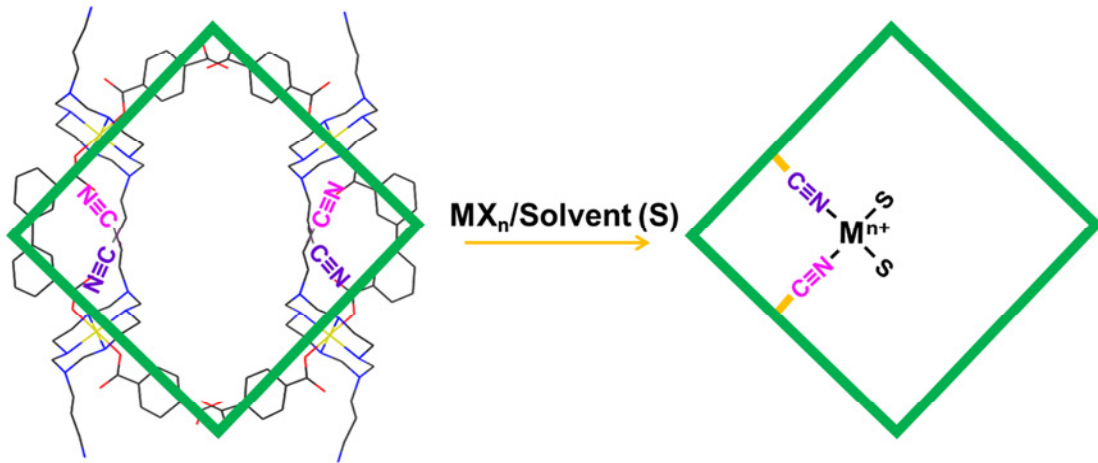
Type: Symposium, Time: WED 14:30, Chair: Ja-Hyoung Ryu

Catalytic Site Anchoring in a Tailored Metal-Organic Framework (MOF)

Sungeun Jeoung, SONG HO LEE, Hoi Ri Moon*

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

Homogeneous transition metal catalysts are many obvious advantages to controlling reaction speed and selectivity under relatively mild operating conditions. However, homogeneous catalysts are difficult to separate from the products and reuse in industry. Because of that, heterogeneous catalysts receive much attention in industrial processes, but they often have some shortcomings in low selectivity, low activity, and tough operating conditions. One of the ways to solve these problems is anchoring of transition metal complexes to inorganic supports. The heterogenization of homogeneous molecular catalysts enhances their stability and reaction scope while maintaining their tunability and activity-selectivity. Herein, we utilize metal-organic frameworks (MOFs) as a heterogeneous support for incorporating transition metal catalysts. Well-designed MOFs are suitable for catalyst due to their high surface areas and porosity. $[\text{NiL}_{\text{CN}}]_2(\text{BPTC})$ has a large pore channel anchoring the transition metal (Cu, Co, Pd, Mn, Ni and Cr), it is used to catalysts for ethylene oligomerization. Linear α -olefins will be synthesized through the ethylene oligomerization, which can be used as intermediates for manufacturing of detergents and lubricants. We expect that transition metal included with $[\text{NiL}_{\text{CN}}]_2(\text{BPTC})$ is a highly active catalyst for ethylene oligomerization.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-2**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 14:40, Chair: Ja-Hyoung Ryu

Defect Engineering for Functionalization of Metal-Organic Frameworks

Seongwoo Kim, Hyojin Park, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs or also called as Porous Coordination Polymers, PCPs) are three dimensional porous materials that are constructed from the assembly of metal ion clusters and organic ligands. MOFs are of great promise materials for a variety of applications such as gas storage, separation, catalysis, etc, because of the near infinite possibilities regarding their structure, porosity, and chemical functionality.^[1]

Recently, structural defects were revealed in MOF crystal structures have many interests in coordination material research fields. Since MOFs are constructed by repeating coordination bonds between metal ions (or clusters) and organic ligands, the disappearance of metal clusters or organic linker molecules generate structural defects on the frameworks.^[2] The structural defects could give physically unstable frameworks, however, at the same time, allow more accessible channel or porosity to the guest molecules. Very recently, the defect engineering in MOFs pores are receiving much attention from this point of view.

In this presentation, our recent efforts for applying defect engineering to functionalization tools of MOFs will be discussed. The existence of defect in the framework could accelerate the diffusion of functionalized molecule and produce the installation of functional molecules. The scope of functionalizations and the detail kinetics along with application will be presented.

References

[1] H.-C. Zhou, J. R. Long, and O. M. Yaghi, *Chem. Rev.*, **2012**, *112*, 673.

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Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-3**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 14:50, Chair: Ja-Hyoung Ryu

Amino acid functionalized Zr-MOF for heterogeneous catalysis and heavy metal adsorption

Hye Hyun Kim, Somi Won, Junmo Seong, Gyoung Hwa Jeong, Myoung Soo Lah*

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

Metal-organic frameworks (MOFs) are a class of microporous materials composed of metal ions and organic ligands through coordination bonding. Open metal sites and functionalized residues at the pore make them promising candidates as heterogeneous catalysts and adsorbents. Recently, Zr-based MOFs such as UiO-66 series, NU-1000 and MOF-808 are spotlighted because of their water stability and chemical reactivity. In MOF-808 with (3,6)-c **spn** net topology, 6-c $[\text{Zr}_6\text{O}_4(\text{OH})_4(\text{COO})_{12}]$ clusters are interconnected by using 3-c trimesic acid (btc) ligands. Only six carboxylates among the 12 carboxylates of the Zr cluster are connected to btc ligands and the remaining six carboxylates are terminating ligands. The terminating carboxylate ligands can be further replaced by other carboxylate ligands including amino acids and their derivatives. For example, the MOF-808 grafted by using cysteine, MOF-808-Cys, can be prepared and used for the selective and efficient captures of heavy atoms such as Cd and Hg ions since the thiol residue of the cysteine has strong binding affinity for soft heavy atoms. The MOF-808 grafted by using other amino acid, MOF-808-Amino, can also be used for biomimetic catalysis such as various hydrolysis and aldol condensation reactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **KCS4-4**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 15:00, Chair: Ja-Hyoung Ryu

A catecholamine neurotransmitter towards pathogenic features found in Alzheimer's disease

Eunju Nam, Mi Hee Lim *

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

Information on interactions between dopamine and multiple pathogenic factors of Alzheimer's disease (AD) [*i.e.*, amyloid- β ($A\beta$), metals, reactive oxygen species (ROS)] is very limited; thus, despite a suggested link of dopamine to AD pathology, it is difficult to elucidate its influence on AD pathogenesis. Herein, we report dopamine's direct interactions and reactivities with both metal-free $A\beta$ and metal-bound $A\beta$, along with its effect on the activation of proteins capable of controlling inflammation as well as oxidative stress. Moreover, our studies of a new chemical library, designed through structural variations of dopamine, identified that dopamine's oxidative cyclization with concomitant ROS production could be essential for controlling $A\beta$ aggregation and $A\beta$ -induced cytotoxicity. Detailed biochemical, biophysical, and biological investigations regarding how dopamine is able to modulate multiple AD pathogenic features will be presented. Our overall studies provide new insight into a novel role of a catecholamine neurotransmitter, dopamine, in AD pathology.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-5**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 15:10, Chair: Ja-Hyoung Ryu

Practical 2D ensemble channels for crystal structure determination of liquid chemicals via SCSC guest exchange

DAYE CHOI, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

The single-crystal-to-single-crystal (SCSC) solvate exchange of $[\text{Ag}_2(\text{CF}_3\text{SO}_3)_2\text{L}_2] \cdot 2\text{C}_4\text{H}_8\text{O} \cdot 2/3\text{CH}_3\text{OH} \cdot 1/3\text{H}_2\text{O}$ ($1 \cdot 2\text{C}_4\text{H}_8\text{O} \cdot 2/3\text{CH}_3\text{OH} \cdot 1/3\text{H}_2\text{O}$) and $[\text{Ag}_2\text{L}_2(\text{C}_4\text{H}_8\text{O})_2](\text{PF}_6)_2 \cdot \text{C}_4\text{H}_8\text{O} (2 \cdot \text{C}_4\text{H}_8\text{O})$ at various temperatures offers a landmark in delicate proof-of-concept experiments on both pore-shape and temperature. **1** and **2** are 2D networks consisting of 54-membered metallacyclic rings in a slightly sliding multi-layered mode with open channels and in a staggered multi-layered mode with closed cages, respectively, forming the single crystals of P- and M-helical enantiomeric multi-layered ensembles. The solvate molecules of **1** in cyclic liquid media are fully exchanged to transform each solvate crystal such as $1 \cdot 3\text{C}_4\text{H}_8\text{O}_2$ from dioxane in a SCSC state. Thus, the crystal structures of various ring compounds such as tetrahydrofuran, dioxane, benzene, cyclohexane, cyclohexene, bromobenzene, cyclohexanol, tetrahydropyran, and... as solvates nestled in the matrix **1** are fully refined and solved. The SCSC solvate exchange of a series of **1** is proportional to temperature. Thus, this stable molecular system **1** is the most efficient reproducible and flexible porous matrix for the crystal structures of various liquid ring compounds in a SCSC state. In contrast, those of $2 \cdot \text{C}_4\text{H}_8\text{O}$ with closed cages are not exchanged even at 70 °C.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-6**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 15:35, Chair: Min Kim

Robust porous superstructure synthesized *via* solid-state reaction

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

²*Division of Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

Solid-state reactions have appealed to the organic synthetic field due to their simplicity, efficiency, and selectivity compared to liquid-phase reactions. Herein, the superstructure was realized by the solid-state reaction which converted single-crystal-to-single-crystal. The superstructure of 5,5',5''-(1,3,5-triazine-2,4,6-triyl)triisophthalonitrile (TIPN) can be formed by cyclotrimerization of 1,3,5-tricyanobenzene (TCB) single crystals. The TIPN superstructure was determined by single crystal X-ray diffraction and visualized by transmission electron microscopy. As the results, the superstructure has hexagonally packed 1-dimensional (1D) channels along the crystal axis. Furthermore, the superstructure arises from interdigitated nitrile interactions in the crystal lattice, and thus has electron-beam tolerance and high thermal stability.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-7**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 15:45, Chair: Min Kim

Replaceable Lewis Acid Catalysts in Surface-modified Metal-Organic Frameworks

Hakyung Yun, Jaheon Kim *

Department of Chemistry, Soongsil University, Korea

A small-mesoporous metal-organic framework (MOF), Cr-MIL-101 has been chemically modified with polar functional groups such as amino acids, $-NH_2$, or $-COOH$, and employed as a host for metal complex guests. To this MOF, pyridines having pendant alcohol groups such as pyridine propanol have been introduced via their H-bonding formation with the framework surfaces and used as new coordinating sites for metal ions that can show Lewis acid catalysis. Since various pyridine alcohols can attach to the framework surface, the platform host is useful for screening potential catalysts for organic reactions in an efficient way. In this presentation, we will explain in detail the synthesis, characterization, and applications of the platform MOF.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-8**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 15:55, Chair: Min Kim

Critical Role of (100) Facets on γ -Al₂O₃ for Ethanol Dehydration: Combined Efforts of Morphology-Controlled Synthesis and TEM Study

Jaekyoung Lee, Ja Hun Kwak^{1,*}

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

¹*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

In this work, the effect of crystal facets on the catalytic behavior of γ -Al₂O₃ was investigated by X-ray diffraction, transmission electron microscopy, temperature-programmed desorption of ethanol, solid-state ²⁷Al NMR, infrared spectroscopy, and ethanol dehydration reaction. A series of platelet γ -Al₂O₃ were synthesized, in which the relative ratio of (100) facets had been systematically increased. Ethylene formation increased with increasing (100) facets, clearly demonstrating the critical role of these facets as active sites for ethanol dehydration on γ -Al₂O₃. This systematic approach is helpful for a better understanding of facet-dependent catalytic properties of γ -Al₂O₃ that arise from the interaction between the supported metal and the crystal facets.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-9**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 16:05, Chair: Min Kim

Enzymatic responsive multifunctional metal organic structure for on command drug release

Kibeom KIM, Tae-Hyuk Kwon¹, Wonyoung Choe^{*}, Ja-Hyoung Ryu^{*}

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

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

Nanosize controlled MOF has attracted much attention as a drug carrier because it has many pores and huge surface area. However, in studies using MOF as a drug delivery system, the Gatekeeper system for controlled drug release has not been performed much and more research is needed. The existing MOF gate keeper systems also depend on passive targeting for cancer cell targets. Therefore, MOF gate keeper system with active targeting system is needed for more effective cancer drug delivery. In this study, combined treatment of chemo and photodynamic therapy is possible using PDN-224 MOF composed of Zr and porphyrin organic linker. In addition, a MOF gatekeeper system has been developed in which hyaluronic acid is coated by coordination bonds with MOF surface Zr ions. This system enabled active targeting and controlled drug release in response to CD44 and HAdase present in cancer cells. Moreover, the combination therapy improves the cancer therapeutic effect and has the ability to efficiently treat multi-drug resistance cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-10**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

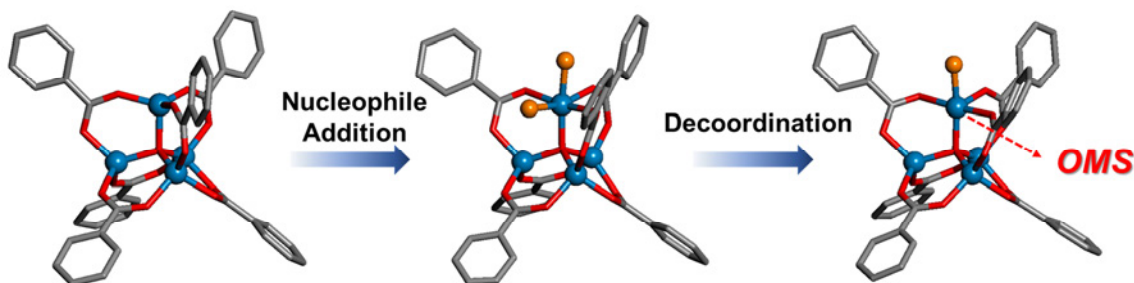
Type: Symposium, Time: WED 16:15, Chair: Min Kim

Solvent-Induced Structural Transitions in a Zn₄O-Containing Doubly Interpenetrated Metal-Organic Framework

Jaehwa LEE, Hoi Ri Moon*

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

Metal-organic frameworks (MOFs), which respond to external stimuli such as guest removal/reintroduction, guest exchange, oxidation, pressure, temperature, and light, vary the chemical or physical properties through the structural rearrangement of their molecular components. Thus, if the transformation occurs in a single-crystal-to-single-crystal (SC-SC) manner, direct observations of structural changes in MOFs are possible through single-crystal X-ray diffraction (SCD). In this context, we present a 3D doubly interpenetrated Zn₄O-containing MOF, which exhibits dynamic structural changes upon guest exchange with organic solvents. Particularly, after the immersion in MeOH over 1 week, one of four tetrahedral Zn²⁺ ions in Zn₄O clusters changes its geometry to octahedral ions with two bound MeOH molecules, which could be crystallographically observed. This unique coordination environment of the SBUs leads the MOF to undergo cation exchange and enable its use in catalytic applications.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-11**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 16:40, Chair: Hoi Ri Moon

The observation of drastic change of metal cluster in metal-organic frameworks by transmetalation

Dongwook Kim, Seok Jeong, Myoung Soo Lah*

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

Metal-organic frameworks (MOF) as crystalline porous material are composed of metal ion or cluster and coordinative organic ligands. MOF are utilized for gas storage or separation, catalyst, sensing due to porosity, diversity and additional tunability to specific purpose. Post-synthetic modification (PSM) method provides an extension of applicability of MOF. PSM can lead to change of its properties or enhancement of quality of MOF with known structures. PSM is also able to induce new materials from existing framework, for example, as attachment of new functional groups, partial exchange of ligands and alternation in metal ion or cluster. Those modification methods give chance to variability, however, the analysis of structural environment about amended product is not easy because deteriorated crystallinity or limitation of analysis condition even though some properties are improved by PSM. So many of PSM-MOF were difficult to investigate structure analysis directly. In this work, we carried out transmetalation of Zn-MOF to Fe³⁺ under ferric chloride solution, then performed single crystal x-ray structure determination about transmetalated Fe-MOF single crystal. This structure determination supplied the observation of change of metal clusters from Zn₄O(COO)₆ to Fe₃O(COO)₆ (with one chloride for charge balance) following Zn²⁺ to Fe³⁺ ion. And we will discuss change of property in those experimental results.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-12**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 16:50, Chair: Hoi Ri Moon

Regioisomeric Controls of Two Functional Groups in Flexible Metal-Organic Frameworks

Hyeon Bin Ha, Kwangho Yoo, Myung Hwan Park¹, Youngjo Kim, Min Kim^{*}

Department of Chemistry, Chungbuk National University, Korea

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

Compare to other porous materials, (e.g. mesoporous silica, zeolites, etc.), the organic functional groups could be installed into the frameworks relatively easily via organic transformations on the organic linker part of metal-organic frameworks (MOFs). This functional groups diversity is one of the great advantages of MOFs.

Recently, we have successfully installed various combinations of two different functional groups in MOF pore. The NH₂-, Cl- (or halogen), MeO-, and NO₂- groups were selectively installed on benzene-1,4-dicarboxylic acid (BDC) with region-selective manners and applied them to MOF synthesis. Very interestingly, the structural flexibility (i.e., breathing behavior of framework) was totally changed by regioisomeric positional controls in some specific combinations. Particularly, we have found that the combinations of NH₂-Cl, NH₂-OMe, OMe-OMe only produced the flexible frameworks when they were placed in para-position.^[1-3]

In this presentation, our recent studied for the physical property changes (i.e., flexible changes or breathing behavior changes) by regioisomerism in MOFs will be summarized and deeply discussed. The structural flexibility changes of MOFs through ligand positioning controls will be presented with ligand synthesis and characterization along with MOF characterizations.

References

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

DOI:10.1039/c7ce00971b.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: KCS4-13

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 17:00, Chair: Hoi Ri Moon

Recombinant protein-MOF hybrid complex

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²*Division of Life Science, Ulsan National Institute of Science and Technology, Korea*

Among the drug delivery carriers, MOF nanoparticle (metal organic framework) have received wide attention due to their tunable pore morphology, high specific surface area, easy surface modification and biodegradability in bio-environment. They can host the therapeutic compounds due their void cores, as extra reservoir for drug storage. Also gatekeeper system can maximize the characterization of MSN for being used drug delivery systems. Although there are many kinds of gatekeeper systems, like polymer, peptide, metal nanoparticles, not much improve in protein gate keeper. Protein gate keeper could be one of the most powerful platform by using direct interaction between receptor protein and affibody. Drug can be loaded into the pores of the carrier at large quantity. Recently, non-covalent protein gatekeepers have received significant attention towards encapsulation stability. Hence, we installed a biocompatible protein gatekeepers on the surface of drug loaded carriers. The GST-affibody possess important role in undergoing degradation in tumor environment. Further, this affibody can be conjugated with different types of antibody to target specific cancer cells to achieve a stable and biocompatible carrier for biomedical applications. Keywords: Glutathione; GST-affibody; Antibody; peptide gatekeepers; MOF nanoparticle, PCN-224; protein corona

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS4-14**

Area: [SRC Symposium] Biomimetic Catalysis Based on Porous Platform (BCP2)

Type: Symposium, Time: WED 17:10, Chair: Hoi Ri Moon

Redox-tuning of Small Molecules to Develop Chemical Regulators for Multiple Pathogenic Elements in Alzheimer's Disease

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¹*School of Life Sciences, Ulsan National Institute of Science and Technology, Korea*

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Various pathogenic factors [*e.g.*, metal ions, metal-free amyloid- β (A β), metal-bound A β (metal-A β), free radicals] are observed to be inter-related leading to the pathogenesis of Alzheimer's disease (AD). In order to regulate their complex interactions, the development of chemical reagents targeting such multiple components has received significant attention. Herein, we report that tuning the redox properties of small molecules is key to inventing effective chemical regulators towards the actions of pathological elements found in AD. In our newly prepared chemical series, **compound 1** with the lowest oxidation potential, is able to modulate the aggregation of both metal-free A β and metal-A β as well as scavenge free radicals. Our biochemical and biophysical studies illuminate that the noticeable reactivities of **1** towards metal-free A β , metal-A β , and free radicals can be achieved *via* peptide oxidation/degradation and ligand oxidation. **Compound 2**, which indicates a relatively higher oxidation potential than **1**, alters Cu(II)-A β_{42} aggregation, whereas **compound 3**, which is hardly oxidized, shows no reactivity with metal-free and metal-treated A β as well as free radicals. Overall, our studies demonstrate that the redox properties of small molecules can determine their regulatory reactivities against multiple factors related to AD pathogenesis.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS5-1**

Area: [Laboratory Safety Education] Study on the Psychological Processes Underlying Errors and Laboratory Management Systems for the Improvement of Chemical Laboratories

Type: Symposium, Time: THU 13:30, Chair: Ik-Mo Lee

Psychological Processes Underlying Human Errors

ChangHo Park

Department of Psychology, Chonbuk National University, Korea

Most of everyday human errors are caused by failures in such psychological processes as attention, memory, and judgment. These psychological processes are involved in various actions in labs, workplace and control rooms, and some failures of which could lead to serious accidents when they are not blocked in the way. Considering psychological mechanisms and their end results different types of human errors can be distinguished, asking different defenses. Reason's (1984) Swiss cheese model can provide a good metaphor in understanding and defending different levels of human errors. Psychological processes at an individual level could be integrated in a causal network of errors in the context of complex systems, as proposed by Senders and Moray (1991). A number of defenses against human errors are discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **KCS5-2**

Area: [Laboratory Safety Education] Study on the Psychological Processes Underlying Errors and Laboratory Management Systems for the Improvement of Chemical Laboratories

Type: Symposium, Time: THU 14:10, Chair: Ik-Mo Lee

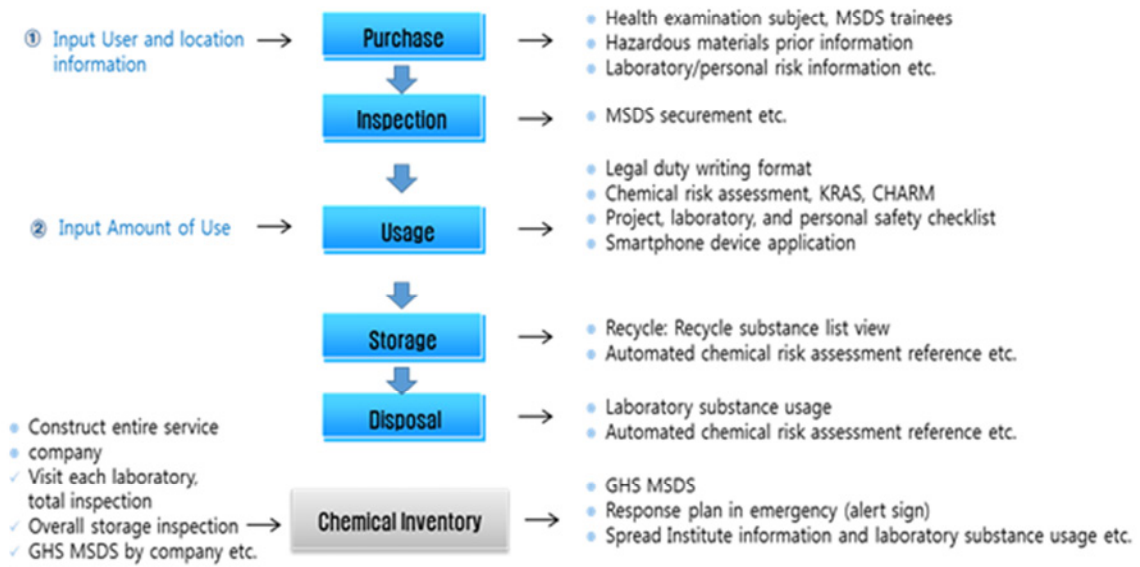
The Development of Chemical Integrated Management System

Young Mi Kim

Korea Research Institute of Chemical Technology, Korea

To reduce chemical risk at laboratory, chemical integrated management systems are developed. Chemicals and safety, health and environmental systems are built synchronously. Various kinds of safety regulatory are provided (Occupational Safety and Health Act, TCCA, research environment Safety Act, Dangerous Goods Safety Management Act, etc.) and improvement may be obtained in both research achievements and researcher's health through dissolving laboratory safety, health and environmental issues. In addition, it is expected that inspiring the importance of both safety and health for the researcher and fluent chemical management could reduce the cost of the damage and accident from laboratory. Overall scheme of chemical integrated management system flow chart is shown in the following figure.

Chemical Integrated Management System Flow Chart



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS5-3**

Area: [Laboratory Safety Education] Study on the Psychological Processes Underlying Errors and Laboratory Management Systems for the Improvement of Chemical Laboratories

Type: Symposium, Time: THU 14:50, Chair: Ik-Mo Lee

KOFWST's Achievements of Safety Management for Women Scientists

Jiyoung Moon

Korea Federation of Women's Science & Technology Associations (KOFWST), Korea

The Korea Federation of Women's Science & Technology Associations (KOFWST), a leading union composed of 59 member organizations in the field of women's science and technology established 'Laboratory Safety Management Committee for Women Scientists' in 2015. The committee aims to spread the need to consider the gender differences in the working environment. Also to change the male-oriented point of view in the Safety Management education curriculum to make a better research environment for men and women in the laboratory and construction sites.

The committee studied whether safety management education curriculum considers the characteristic of women (pregnancy, breastfeeding, or menstruation) within the laboratories. But insufficient of educational materials of showing how to consider the gender differences, especially about the characteristic of women led the committee to publish a guideline for laboratory safety management.

Based on the guideline, the committee published pamphlets and online educational videos. These materials were distributed to universities, research institutes, academies and KOFWST member organizations. Furthermore, the committee held a UCC competition to raise the awareness of safety management issues in the laboratory environment. These ongoing efforts will promote gendered innovations in the field of science and technology.

120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS6-1**

Area: Directions of Basic Research Supports from NRF in Year 2018 and Samsung Research Funding for Future Technology

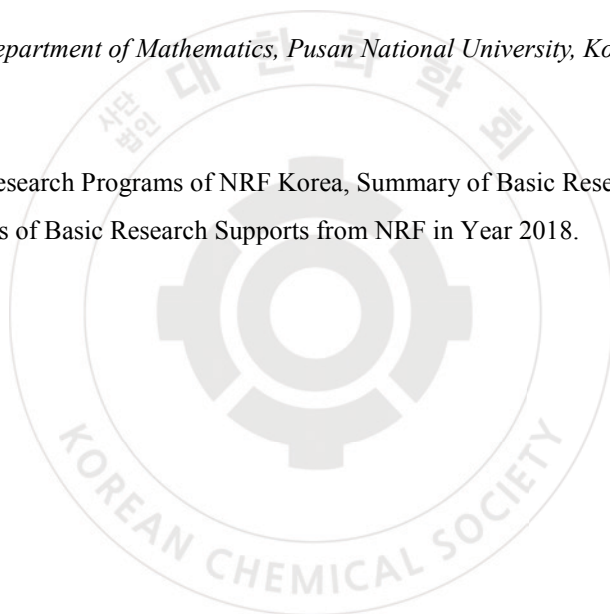
Type: Symposium, Time: FRI 13:00, Chair: Kye Chun Nam

Directions of Basic Research Supports from NRF in Year 2018

Yong-Hoon Lee

Department of Mathematics, Pusan National University, Korea

Introduction to Basic Research Programs of NRF Korea, Summary of Basic Research Supports from NRF in Year 2017, Directions of Basic Research Supports from NRF in Year 2018.



120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **KCS6-2**

Area: Directions of Basic Research Supports from NRF in Year 2018 and Samsung Research Funding for Future Technology

Type: Symposium, Time: FRI 13:40, Chair: Kye Chun Nam

Samsung Research Funding for Future Technology

Sung Hong Kwon

Samsung Electronics Co., Ltd., Korea

TBA



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-1**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 14:30, Chair: Hyeonseok Yoon

Metal-Catalyzed Functionalization of Polymer Surface for Microfluidic Applications

chinnadurai satheeshkumar, Myungeun Seo*

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

The chemical society has been witnessing great advances in functionalization and coupling of organic molecules by using transition metal catalysts in recent years. However, application of such well-developed catalysts in other areas such as polymer chemistry have been relatively scarce despite of huge potential of functionalizing and modifying existing polymers in a tailor-made fashion. Particularly, delicate functionalization of polymer surface using metal catalysts is expected to be highly efficient and beneficial. Here we show such functionalization is possible for parylene, which is chemical vapor-deposited poly(p-xylylene) as a high-performance polymer coating with many superior properties used from satellites in outer space to implantable medical devices and microfluidic devices. We will discuss development of reaction routes based on solution reaction results and characterization of functionalized parylene surface using a variety of analytical techniques. Finally, we will demonstrate use of the functionalized parylene surface for microfluidic applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.O-2**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 14:45, Chair: Hyeonseok Yoon

The Study on Asymmetric Alkyl Substitution and Application to Hole Transporting Materials for Perovskite Solar Cells

Junwoo Lee, Gyeong Ho Kang, SUNG YUN SON, Taiho Park*

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

Existing hole transport material in perovskite solar cells has only been applied to toxic solvents such as chlorobenzene due to solubility problems. These solvents result in limitation for the practical use. Therefore, substitution to non-halogen solvents is important to commercialize of perovskite solar cell devices. Here, we studied on asymmetric alkyl substitution to approach high efficient HTMs with green processing. The concept resulted in asymmetry in the monomer itself, leading to irregularity despite being a homopolymer. Amorphous nature from irregularity is one of the method to increase solubility and miscibility. We synthesize and characterize asymmetric polymer named asy-PBTBDT and fabricate hole transport layers using applicable green solvents from Hansen solubility parameters. The green solvent is named 2-methyl anisole that is used in food additives, which is edible and no harmful in human body. The device using asymmetric polymer leads to a PCE of around 20 % using food additive solvent (2-MA) with additives (Li-TFSI and t-BP) and a PCE of 18 % without additives. Furthermore, the polymeric HTM leads to longer stability than common spiro-OMeTAD. The polymeric HTM may be a promising material to replace spiro-OMeTAD due to a green processing process for commercialization, stability and high efficiency.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-3**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 15:00, Chair: Hyeonseok Yoon

Redesigning the PEG Surface of Nanocarriers for Tumor Targeting

Yoonkyung Kim

Korea Research Institute of Bioscience and Biotechnology (한국생명공학연구원), Korea

Achieving accurate and efficacious tumor targeting with minimal off-target effects is of paramount importance in designing diagnostic and therapeutic agents for cancer. In this respect, nanocarriers have gained enormous popularity because of their attainable multifunctional features, as well as tumor-targeting potential by extravasation. However, once administered into the bloodstream, nanocarriers face various *in vivo* obstacles that may significantly impair their performance needed for clinical translation. Here, we demonstrate a strategy to enhance tumor-targeting efficiency by embedding functionalities in the interior region of partially PEGylated nanocarriers (*ca.* 10 nm in diameter) intended for active or passive targeting. The cooperative impact of these topologically inner functional groups (IFGs) was marked—enhancements of >100-fold in IC_{50} *in vitro* (*e.g.*, a high-avidity ligand with cationic IFG) and >2-fold in tumor accumulation at 2 h post-injection *in vivo* (*e.g.*, a high-avidity ligand with anionic IFG), both against the fully PEGylated counterpart. Analogous to allosteric modulators, properly employed IFGs may substantially improve the process of effectively directing nanocarriers to tumors, which is otherwise solely dependent on avidity or extravasation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-4**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 15:15, Chair: Hyeonseok Yoon

Nanocrystalline cellulose-derived stimulus-responsive cholesteric microgels having catalytic properties

Sangho Cho

Korea Institute of Science and Technology, Korea

Polymer microgels which have a network structure swollen in a solvent are an important class of soft matter materials with variety of potential applications including drug delivery vehicles, sensors, photonic crystals and etalons, microreactors, cell culture media, and separation and purification technologies. Nanofibrillar hydrogels shows interesting properties such as nonlinear viscoelastic behavior, good transport due to large pore size and thermal stability. Particularly, rod-like cellulose nanocrystals (CNC), one of nature-derived filament-like nanoparticles, are attractive building blocks for hydrogel assembly with their surface functionalities and the ability to form cholesteric (Ch) liquid crystalline phase. Recently, we reported nanofibrillar, composite stimulus-responsive CNC-derived microgels with a Ch structure. Microgels with a narrow size distribution were prepared by microfluidic emulsification, followed by the photopolymerization of the precursor droplets. The spherical confinement of CNC led to the liquid crystalline morphology altered from the spherical concentric to the bipolar planar Ch structure by reducing the droplet dimensions. The microgels exhibited collective properties of CNCs and polymer hydrogels. The stimulus-responsive nature of the microgels was governed by the polymer component and was evidenced by tuning the microgel size and pitch at varying ionic strength and temperature of the ambient medium. The microgels exhibited catalytic performance in a hydrolysis reaction and were used for the in situ synthesis of plasmonic AgNPs. The resulting AgNP-laden microgels exhibited catalytic activity in a reduction reaction. In this presentation, design, synthesis, and performance of the composite microgels for catalytic activities will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-5**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 15:30, Chair: Changsik Song

UV-mediated synthesis of thermoresponsive alginate hydrogels and tuning their responsive properties

Eun Jung Choi, Changsik Song^{*}, Ju Hyen Lee, TaeWoo Kim¹

Department of Chemistry, Sungkyunkwan University, Korea

¹*Sungkyunkwan University, Korea*

Stimuli-responsive polymers, which can change their microstructures triggered by environmental stimuli, can be used in shape memory materials because of the fact that the structural changes from the external stimuli can be recovered to their original shapes in a controllable manner. Sodium alginate is one of polysaccharides that can be easily functionalized by several coupling reactions such as amination to carboxylate groups. Also, sodium alginate is well-known for capturing divalent ions giving rise to gelation. In this study, allyl-functionalized alginates were synthesized and subsequently *N*-isopropylamine (NIPAM)-containing alginate hydrogels were prepared by UV-mediated crosslinking via radical reaction. The pNIPAM-crosslinked alginate hydrogels showed different swelling ratios depending on the amount of NIPAM, pH, temperature and several metal cations. The morphology of the hydrogels was investigated by SEM images. Also, the ion-promoted crosslinking showed shape-programming properties with temperature cycling. Several analytical techniques such as IR and rheology were attempted to elucidate the mechanism of shape memory

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.O-6**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 15:45, Chair: Changsik Song

Diaziridine-based Curing Resins for Overcoming Limitations of Epoxy Materials

Seohyun Kang, Hyo Jae Yoon *

Department of Chemistry, Korea University, Korea

This presentation will describe a new class of curing resins based on three-membered *N*-heterocycle, aziridine. Increased complexities in applications involving curable polymers virtually need new materials that can overcome the limitations of existing ones. A series of curing resins, the structure of which is based on three membered *N*-heterocycle—aziridine—have been synthesized, and their thermal curing ability in solution and solid-state were investigated. The results reveal that the chemical reactivity of the aziridine-based curing resins is fine-tunable by controlling the *N*-substituent of aziridine. These curing resins undergo ring-opening polymerization under unprecedentedly mild conditions and show remarkably rapid curing rate, wide substrate scope and excellent chemoselectivity, as compared to the analogous epoxy agents.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-7**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 16:00, Chair: Changsik Song

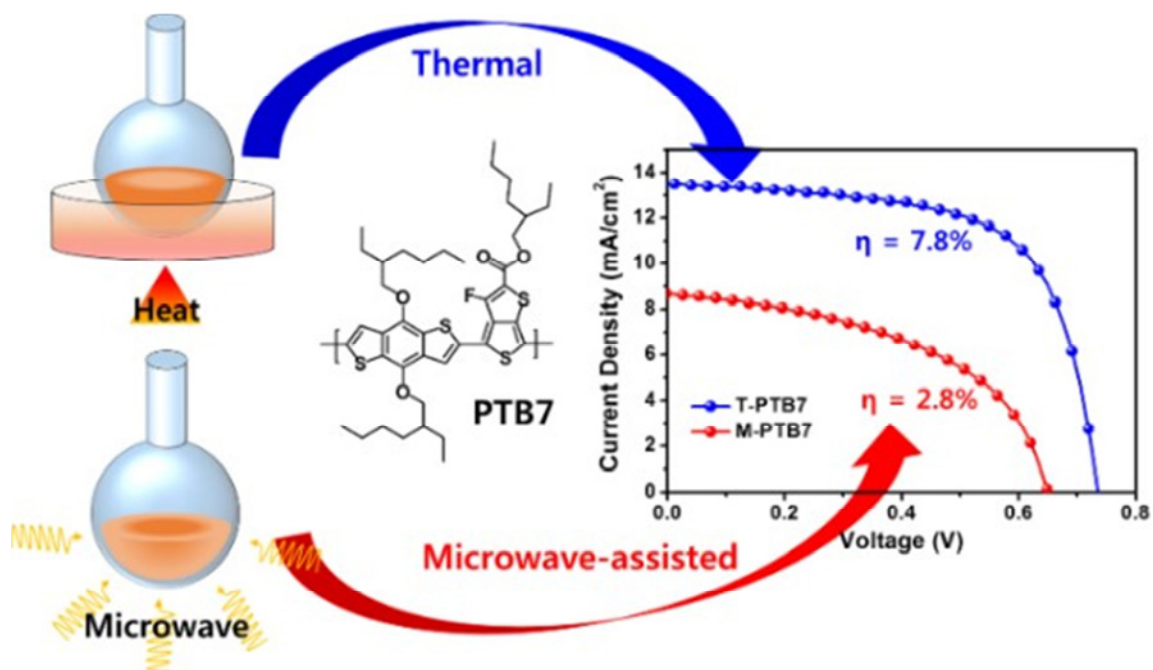
Effects of microwave-assisted polymerization on the photovoltaic performance of PTB7 solar cell

Minjun Kim, HONG IL KIM¹, Sangwon Kim¹, Taiho Park^{1,*}

Chemical engineering, Pohang University of Science and Technology, Korea

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

We report effects of microwave-assisted polymerization on the photovoltaic performance of polymer solar cell using benzodithiophene-based polymer (PTB7) as a donor material. For systematic and comparative study, we synthesized PTB7 polymers through Stille-coupling polymerization under microwave conditions (M-PTB7, $M_n = 75 \text{ kg mol}^{-1}$, and $D = 2.2$) as well as thermal conditions (T-PTB7, $M_n = 31 \text{ kg mol}^{-1}$, $D = 2.1$). Although the microwave-assisted polymerization is a powerful method to increase the M_n of PTB7 without broadening D in a short time, this method decrease the power conversion efficiency from 7.8% (T-PTB7) to 2.8 % (MPTB7). We found that the microwave-assisted polymerization accelerates more structural defects from homo-coupling side reactions, resulting in a significant decrease in JSC and FF values for M-PTB7. The increased abundance of these homo-coupled units under the microwave-assisted conditions was demonstrated by various optical spectroscopy methods and the model reaction study.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.O-8**

Area: Oral Presentation for Young Scholars in Polymer Chemistry

Type: Oral Presentation, Time: FRI 16:15, Chair: Changsik Song

Control of the Donor/Acceptor Interfacial Morphology via Quadrupolar Electrostatic Interactions for All-Polymer Solar Cells

HONG IL KIM, Minjun Kim¹, Cheol Woong Park, Taiho Park*

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

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

We report a pentafluorobenzene-based additive (FPE) to control the donor/acceptor (D/A) interfacial morphology via quadrupolar electrostatic interactions between donor and acceptor polymers in all-polymer solar cells (all-PSCs). The morphology changes are investigated using a combination of atomic force microscopy (AFM), grazing incidence wide-angle X-ray scattering (GIWAXS), and near-edge X-ray absorption fine-structure spectroscopy (NEXAFS). Unlike a conventional solvent additive, such as 1,8-diiodooctane (DIO), a bicontinuous interpenetrating morphology without large-scale phase separation and an enhanced π - π stacking with face-on orientation are found in the FPE processed blended films. These morphology changes improve the charge carrier extraction and charge transport between D/A interfaces to achieve an increase in the photovoltaic performance of all-PSCs.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.O-1**

Area: Oral Presentation of Young Inorganic Chemists

Type: Oral Presentation, Time: THU 09:00, Chair: Won Cheol Yoo

Carbon dioxide Working Capacity Control in Heterodiamine-Functionalized Metal-Organic Frameworks

Woo Ram Lee^{*}, Chang Seop Hong^{1,*}

Department of chemistry, Sejong University, Korea

¹*Department of Chemistry, Korea University, Korea*

The biggest crisis facing mankind today is global warming which causes extreme climate change and eustatic sea level rise. The combustion of fossil fuel causes raising atmospheric CO₂ concentration which is major source of greenhouse effect. To effectively capture the CO₂, our investigation focused on synthesizing practical CO₂ capture materials like MOFs. In this work, we report synthesis, CO₂ adsorption, working capacity, adsorption mechanism and chemical or physical stability of new type of heterodiamine functionalized MOFs for CO₂ capture. To fully amine functionalize, we successfully synthesized extended version of MOF-74 which have 18.9 Å wide channels. After which we synthesized via postmodification Heterodiamine-functionalized metal-organic framework (MOFs), men'-Mg₂(dobpdc), een-Mg₂(dobpdc) and ipen-Mg₂(dobpdc) (men'=N-methylethylenediamine, een = N-ethylethylenediamine, ipen = N-isopropylethylenediamine), which contain heterodiamines with primary and secondary amines. High working capacities are achieved at low regeneration temperatures. And these adsorbents have useful CO₂ capture working capacities and good stability under humid conditions. These MOFs can be hopeful adsorbent for practical post-combustion CO₂ capture process.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.O-2**

Area: Oral Presentation of Young Inorganic Chemists

Type: Oral Presentation, Time: THU 09:30, Chair: Won Cheol Yoo

Methods for Controlling Properties and Functions of Organic and Inorganic Materials

Jin Kuen Park

Department of Chemistry, Hankuk University of Foreign Studies, Korea

My research interest is centered on the molecular design and synthesis of innovative, functional materials for applications in organic electronics (including, for example, conjugated small molecules and polymers for organic photovoltaics and field-effect transistors). In addition to the synthetic foundations, I am also focused on contributing to the fundamental understanding how material's molecular structures can affect their optical, electronic properties, and molecular packing behavior with the objective of being able to guide the future design of high-performance and high-efficiency organic devices. Besides, I have developed synthetic methods for the preparation of hybrid materials consisting of inorganic/organic constituents. Especially, the inorganic/organic hybrids based on two dimensional inorganic lattice such as layered double hydroxides (LDHs) and functional polymers have been studied to tailor the desirable physico-chemical properties of such hybrids.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.O-3**

Area: Oral Presentation of Young Inorganic Chemists

Type: Oral Presentation, Time: THU 10:00, Chair: Won Cheol Yoo

Application of Electrochemical Methods in Artificial Photosynthesis

Hyun Seo Ahn

Department of Chemistry, Yonsei University, Korea

Conversion of solar energy into transportable liquid fuels has been an important research theme in physical sciences for the last decade. Many artificial photosynthetic devices have been built with numerous iterations and enhancements, yet all fall short of the biological machinery. In the current presentation, two major problems in artificial photosynthesis will be discussed: 1) limited lifetime of the photo-absorber due to oxidative degradation and 2) deficient understanding of the complex oxygen evolution reaction (OER). In the first part of the presentation, a proof-of-concept photo-anodic device for OER will be demonstrated. Prolonged use of corrosion sensitive n-type silicon was made possible in water by application of an electrodeposited thin passivating layer of TiO₂. A rare metal/insulation/semiconductor junction was employed for solution electrochemistry; insights into the tunneling electron transfer phenomenon involved in solution chemistry will be presented. In the second part of the talk, an investigation of the catalytic OER surface processes will be presented. By use of a redox titration experiment, the redox processes occurring at the surface of metal oxides during OER were investigated.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.O-4**

Area: Oral Presentation of Young Inorganic Chemists

Type: Oral Presentation, Time: THU 10:30, Chair: Won Cheol Yoo

Inorganic nanoparticle regulates bone metabolism

Shin-Woo Ha

Department of Radiology, Seoul National University Bundang Hospital, Korea

Osteoporosis is to decrease bone density caused by hormone change after menopause or aging. Bone becomes fragile and easily breaks up by minor impact. According to the statistics by Health Insurance Review & Assessment Service osteoporotic patients are largely increased because of rapid aging in the population. In 2015, total 821,754 people diagnosed osteoporosis, and among them 93.4% was women. There was a significant difference in gender. Bisphosphonate derivatives, which are catabolic and prevent bone loss are used for the treatment of osteoporosis at the present. Osteonecrosis of the Jaw (ONJ) can occur when a patient has a long treatment of the bisphosphonate. Therefore, the development of an anabolic agent to promote bone mineralization is necessary. Recently we developed two types of inorganic nanoparticles; silica-based nanoparticles (NPs) and nano-hydroxyapatite (nano-HAp). We showed that silica-based NPs stimulate the differentiation of osteoblasts, bone-forming cells and mineralization, and suppress the differentiation of osteoclasts, bone-resorbing cells. In in-vivo study, young mice increase bone mineral density (BMD) and old mice inhibit to decrease BMD. The other, nano-HAp is composed of the same composition of bone, calcium and phosphates. When nano-HAp were exposed to osteoblasts, alkaline phosphatase (ALP), which modulates mineralization was strongly suppressed. Even nano-HAp didn't internalize into the cell, but contacted on the cell surface and stimulated a cell signaling pathway. We proposed that the regulation of ALP expression resulted from DNA methylation by nano-HAp.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-1**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 09:00, Chair: Sang-Yong Ju

High-throughput simulations and single-molecule experiments reveal DNA looping and self-association controlled by sequence and methylation

Jejoong Yoo, Sangwoo Park¹, Taekjip Ha¹, Aleksei Aksimentiev^{2,*}

Center for self-assembly and complexity, Institute for basic science, Korea

¹*Johns Hopkins University, USA, United States*

²*University of Illinois at Urbana-Champaign, United States*

Human chromosomes have long been thought to behave like random polymers encapsulated in a nuclear envelop. However, it is becoming more and more clear that that chromosomes organize into certain three-dimensional structures that dynamically change depending on the cell's state. The very presence of such structures implies that yet unknown physical interactions govern the free energy change in the process of cell development and cancer. To find a clue about the mystery, we determined the free energy landscape of a nucleosome---the fundamental structural unit of chromosome that consists of a fragment of DNA wrapped around a protein core. Technically, we combined high-throughput molecular dynamics simulations and single-molecule experiments. At a single nucleosome level, we found both sequence and CpG methylation of DNA to uniquely determine the orientation of the DNA loop with respect to the protein core. This finding offers a simple physical mechanism of controlling DNA accessibility to RNA polymerases. At a multi-nucleosome level, we found the AT content of the DNA sequence and the methylation of either DNA or the nucleosome proteins to govern association of nucleosomes into clusters. Overall, our findings suggest that DNA is a remarkable polymer that can program its own free energy landscape by sequence and methylation to regulate the nucleus-scale organization of chromosomes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-2**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 09:10, Chair: Sang-Yong Ju

Structural transformations on the bond fission dynamics of 2-methoxythiophenol-d₁

Jean Sun Lim, Sang Kyu Kim *

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

Bond fission dynamics of 2-methoxythiophenol-d₁ (C₅H₅OCH₃SD) has been investigated in the first excited state by velocity map imaging method. The photofragment D atom was detected and their low and high total kinetic energy release (TKER) distributions correspond to the ground (\tilde{X}) and excited (\tilde{A}) state of the cofragment 2-methoxythiophenoxy radical. At band origin of the first excited state, the striking \tilde{X}/\tilde{A} ratio of the photoproducts was observed in comparison with the ratios of other thiophenol derivatives [1]. This result was quite surprising because the electronic excitation to the first excited state ($\pi\pi^*$) induces structural change from planar to nonplanar and thus a low \tilde{X}/\tilde{A} ratio was expected. It indicates that the molecule adopts planar structure on the dissociative $\pi\sigma^*$ potential energy surface and passes the $\pi\sigma^*/S_0$ conical intersection. The relax scan on the first excited state along the S-H bond length supports the explained dynamics. The intramolecular hydrogen bonding between the hydrogen and oxygen in the methoxy group would play a major role in the dissociation dynamics. As increasing the excitation energy, the adiabatic pathways (with nonplanar structure) become active as internal energy increases. Reference 1. Songhee Han, Hyun Sik You, So-Yeon Kim, and Sang Kyu Kim, J. Phys. Chem. A. 118, 6940 (2014).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-3**

Area: Oral Presentation for Young Scholars in Physical Chemistry

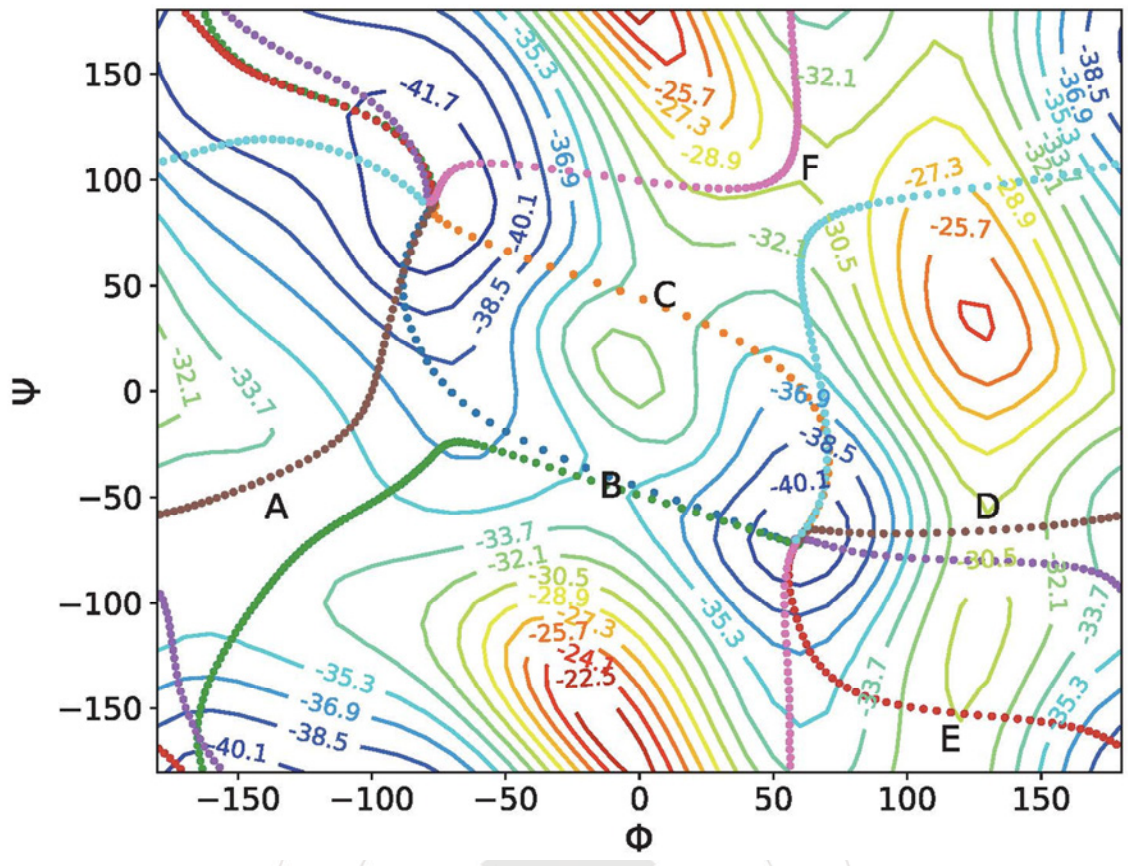
Type: Oral Presentation, Time: THU 09:20, Chair: Sang-Yong Ju

Finding multiple reaction pathways via global optimization of action

Juyong Lee

Department of Chemistry, Kangwon National University, Korea

We present a new computational approach, Action-CSA, to sample multiple reaction pathways with fixed initial and final states through global optimization of the Onsager-Machlup action using the conformational space annealing method. This approach successfully samples not only the most dominant pathway but also many other possible paths without initial guesses on reaction pathways. Pathway space is efficiently sampled by crossover operations of a set of paths and preserving the diversity of sampled pathways. The sampling ability of the approach is assessed by finding pathways for the conformational changes of alanine dipeptide and hexane. The benchmarks demonstrate that the rank order and the transition time distribution of multiple pathways identified by the new approach are in good agreement with those of long molecular dynamics simulations. We also show that the lowest action folding pathway of the mini-protein FSD-1 identified by the new approach is consistent with previous molecular dynamics simulations and experiments.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-4**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 09:30, Chair: Sang-Yong Ju

A Mechanism at a Molecular Level for the Shear Exfoliation of Nanoplates

Inhyuk Jang, Bong June Sung^{*}

Department of Chemistry, Sogang University, Korea

Graphene is one of promising materials with various potential applications due to its unique properties. One of stumbling blocks to the application of graphene would be that it is difficult to prepare a large amount of single layer graphene from graphite without worsening its desired properties. Recent studies suggested that when a shear force was introduced to the graphene nanosheets, quite a monodisperse distribution of graphene could be prepared. However, scientific questions still remain: how the shear would be delivered effectively to the graphite and how the shear would be sufficient to overcome the strong van der Waals interactions between layers of graphene. In this work, we perform extensive non-equilibrium molecular dynamics simulations to answer those scientific questions. We employ a simple model for two layers of nanoplates to mimic the graphene with an explicit solvent model. A steady shear experiment is realized in our simulations by confining solvent molecules and nanoplates between two walls and moving an upper wall at a constant velocity. We find that the interaction between solvent molecules and nanoplates matters: as the interaction becomes more attractive, a larger shear would be required for the exfoliation. We construct a pseudo-phase diagram for the exfoliation as a function of the shear rate and intermolecular interaction. We also find that the shear exfoliation process consists of several steps, each of which corresponds to the barrier crossing in the free energy profile. This suggests that the shear exfoliation is not a single step that overcomes a huge van der Waals energy barrier but is a complicated process that follows the minimum path along the free energy landscape. A detailed molecular mechanism will be also discussed in this talk.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-5**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 09:40, Chair: Sang-Yong Ju

Preparing Highly Luminescent Gold Nanoclusters via Surface Modification

Kyungrim Pyo, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Quantum-sized gold nanoclusters (AuNCs) with photoluminescence properties have been actively studied as a promising material for optical and biological applications. However the uncertainty about the origin of the luminescence properties and the low quantum yield (QY₂₂SG₁₈ (Au₂₂, QY~7%) via relevant surface modification. Firstly, Au₂₂ was ion-paired with bulky tetraoctylammonium (TOA) cation that binds with carboxylate anions of glutathione, which rigidified the Au(I)-shell structure by significant intermolecule interactions between the alkyl chains of TOA cations. TOA-Au₂₂ was confirmed to maintain its composition, while the quantum yield showed a mass increment of 9-fold enhanced luminescence (QY~60%). This is one of the highest reported so far for gold nanoclusters. However the clusters are not soluble in water which limits their use in biological applications. Therefore secondly, we prepared a Au₂₂ whose surface was engineered with benzyl chloroformate and pyrene (Py) to achieve higher quantum efficiency in water. This strategy not only enhanced the luminescence by more than 5-fold (QY~30%) in water, owing to the rigidifying effect of the aromatic molecules, but also induced resonance energy transfer from Py to Au₂₂ when photoexcited at 350nm. As a result the pyrene functionalized Au₂₂ cluster showed 8-fold increased luminescence compared to Au₂₂. These strategies open up a new way for preparing highly luminescent non-toxic AuNCs for optical and biological applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-6**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 10:00, Chair: Sang-Yong Ju

Target-based drug discovery through inverse quantitative structure-activity-lipophilicity relationships and molecular simulation

**Petar Zuvela, Jay Liu^{1,*}, Myunggi Yi², Paweł Pomastowski³, Gulyaim Sagandykova⁴,
Tomasz Bączek⁵, Jarosław Sławiński⁶, Ming Wah Wong, Bogusław Buszewski³**

Department of Chemistry, National University of Singapore, Singapore

¹*Department of Chemical Engineering, Pukyong National University, Korea*

²*Department of Biomedical Engineering, Pukyong National University, Korea*

³*Department of Environmental Chemistry and Bioanalytics, Nicolaus Copernicus University, Poland*

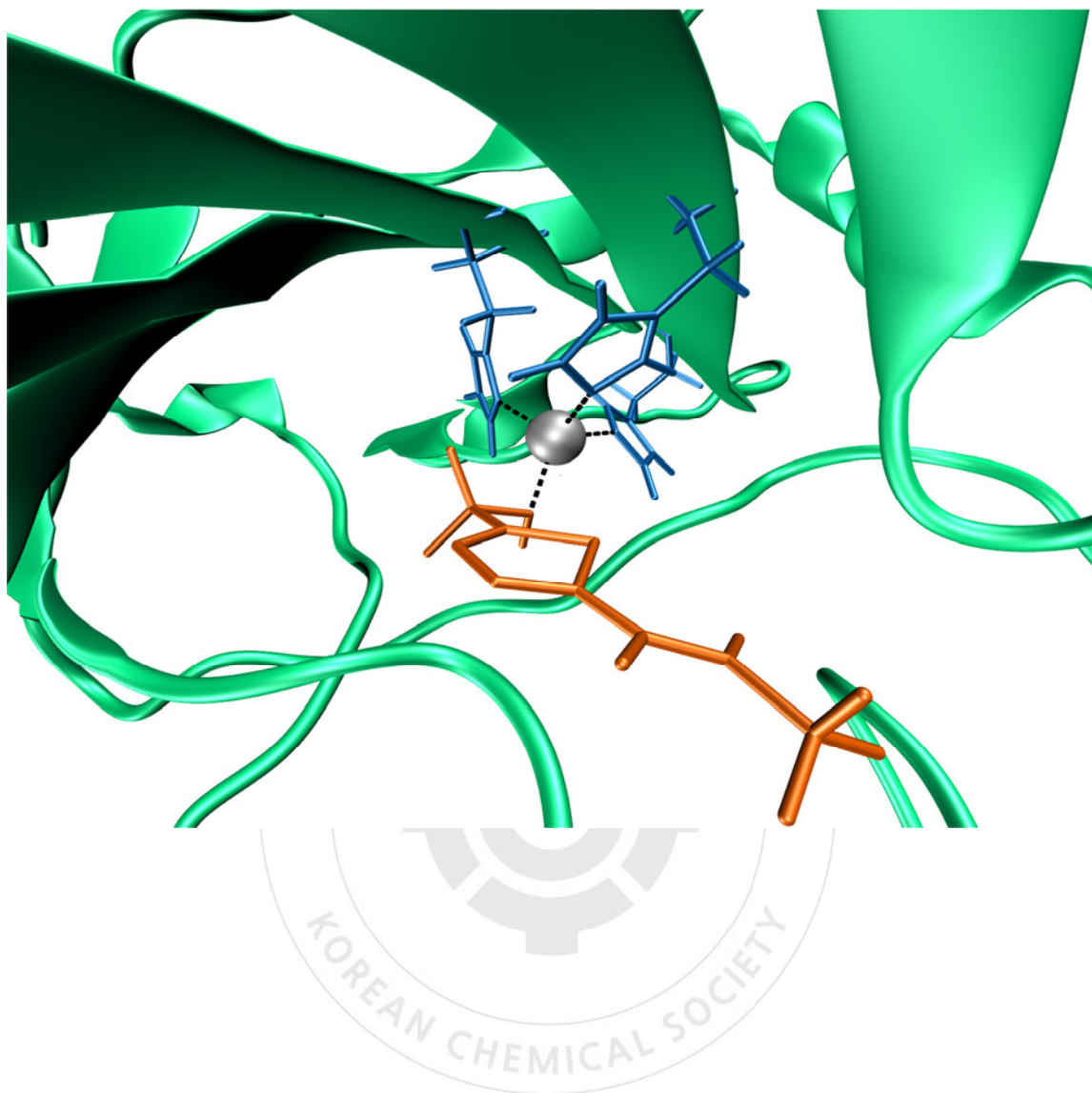
⁴*Nicolaus Copernicus University, Department of Environmental Chemistry and Bioanalytics, Poland*

⁵*Department of Pharmaceutical Chemistry, Medical University of Gdańsk, Poland*

⁶*Department of Organic Chemistry, Medical University of Gdańsk, Poland*

If drug properties are a function of its molecular structure, then the ideal drug candidate's molecular structure is an inverse function of their maximum. This is the reasoning behind a drug discovery methodology presented in this work. As a model system, 45 sulfonamide derivatives in complex with carbonic anhydrase IX (CA IX) were used for development of strongly predictive quantitative structure-activity-lipophilicity relationships (QSALR) model. The model was reversed through numerical optimization in order to obtain an optimal molecular structure, in respect to a reference sulphonamide. Simultaneously, eight testing ligands were complexed with CA IX and characterized experimentally. Gel electrophoresis and MALDI-TOF/TOF-MS were used to determine the mass of the enzyme and explore the dimerization of CA IX. RP-LC and stopped-flow spectrophotometry were used for determination of lipophilicity and inhibitory activity, respectively. FTIR was used to elucidate the structural changes between the recombinant CA IX and its complexes. Molecular dynamics (MD) simulations were performed to complement the experiments, and vice-versa. Results have shown that upon simulation of acetazolamide in complex with CA IX, the system conserved the experimental flexibility profile, and the average radius of gyration obtained by MD analysis agreed well with its empirical value. MALDI-TOF-

TOF/MS has confirmed strong binding of inhibitors to CA IX, while subtle weaker interactions between the ligands and CA IX were elucidated with spectroscopic experiments and MD analysis.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-7**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 10:15, Chair: Sang-Yong Ju

Conformer-specific vibrational spectroscopy of molecular cations by high-resolution VUV-MATI technique

Yu Ran Lee, Hong Lae Kim, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

We have developed the high-resolution vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectrometer. Basically, key ideas on construction of the spectrometer with high-performance was a new ion source assembly consisting of a separate pulse field ionization (PFI) stage to improve the spectral resolution in the VUV-MATI spectrum and a dual stage extraction to achieve the first-order focusing of the MATI ions generated initially with the spatial distribution. This concept on instrumentation could be rationalized by utilizing the SIMION program (3D 7.0w, Win NT) which is used to calculate trajectories of charged particles by electric potentials for various configuration of the electrodes with the voltage. Thereafter, the ion source assembly was optimized at a specific configuration with four electrode plates. In the new ion source, the one stage is for applying a low PFI voltage and the other is for achieving the first-order space focusing of the MATI ions generated. This simple modification in the electrode assembly and the pulsing scheme allowed to enhance simultaneously the spectral resolution ($\sim 8 \text{ cm}^{-1}$) and strength of the MATI signal. In addition, the stability of the vacuum ultraviolet radiation generated by four wave difference frequency mixing in Kr was tremendously enhanced by increasing the volume of the Kr cell and effectively evacuating it. The excellent performance of the constructed VUV-MATI spectrometer has been ensured elucidating complicated vibrational structures of the pyridine cation and the 2-fluoropyridine cation. We also determined the accurate ionization energies and conformational structures of saturated heterocyclic molecules such as thietane, tetrahydro- thiophene, and aldehydes such as isobutanal, which play an important role in biological systems and interstellar media. Vibrational assignments of the observed VUV-MATI spectra could almost completely be achieved by simulating with the Franck-Condon factors and vibrational frequencies calculated adjusting geometrical parameters of the cationic conformers with the DFT method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-8**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 10:30, Chair: Sang-Yong Ju

A series of DFT studies on TiO₂ nanoparticles with a modified hybrid functional

Kyoung Chul Ko, JIN YONG LEE*

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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] In this talk, a series of DFT studies on TiO₂ nanoparticles using this PBEx functional will be briefly presented to introduce examples of its practical application. The properties of single oxygen vacancies of (TiO₂)₃₅ as a prototype of reduced nanoparticle, [2] the properties of anatase nanoparticles in the 1-6 nm size range [3] and the prediction of size dependent band alignment in anatase and rutile nanoparticles [4] will be discussed. The present approach may provide a sufficiently accurate way to study the electronic structure of large TiO₂ nanoparticles which consist of hundreds or thousands of atoms where GW techniques are unaffordable. References [1] K. C. Ko, O. Lamiel-García, J. Y. Lee and F. Illas Phys. Chem. Chem. Phys. 2016, 18, 12357. [2] S. Kim, K. C. Ko, J. Y. Lee and F. Illas Phys. Chem. Chem. Phys. 2016, 18, 23755 [3] O. Lamiel-García, K. C. Ko, J. Y. Lee, S. T. Bromley and F. Illas J. Chem. Theory. Comput. 2017, 13, 1785 [4] K. C. Ko, J. Y. Lee, S. T. Bromley and F. Illas, manuscript preparation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.O-9**

Area: Oral Presentation for Young Scholars in Physical Chemistry

Type: Oral Presentation, Time: THU 10:45, Chair: Sang-Yong Ju

Why is the photo-induced intersystem crossing of ruthenium(II) complex ultrafast and efficient?

JUNWOO KIM, Taiha Joo*

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Highly efficient photosensitizing property of transition-metal (TM) complexes has been exploited for various applications such as photovoltaic devices and photo-catalysts. For the charge generation process to occur efficiently in such systems, electron donor must be highly populated and have longer lifetime than the charge generation time. TM complexes satisfy these conditions, as their triplet states are populated by ultrafast intersystem crossing (ISC) with extremely high quantum yield. High spin-orbit coupling (SOC) constant of TM complexes leads to the ultrafast ISC, which can be measured directly by fluorescence decay. Photophysical properties of tris(2,2'-bipyridine)ruthenium(II) (RB) have been studied extensively as a typical system of TM complexes. Although, the ultrafast ISC of Ru(II) complex has been widely studied by various spectroscopic methods, it is still unclear because of its ultrafast reaction time, which is estimated to be shorter than 50 fs. To investigate the ultrafast ISC of Ru(II) complex, we studied RB and three RB analogs by time-resolved fluorescence (TRF), transient absorption (TA), and DFT/TD-DFT calculations. Time resolutions of TRF and TA were 60 and 25 fs, respectively. We measured accurate ISC times and the photo-induced coherent nuclear wave packets of all four samples, in which the vibrational motion, symmetry, and SOC are distinct. Interestingly, the calculation and experimental results classify the four complexes into two groups. The classification into the two groups and their electronic and vibrational features reveal the correlation between the ISC and nuclear motion and the details of the ultrafast ISC mechanism.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-1

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:00, Chair: Wonryeon Cho

Application of Powder X-ray Diffraction Technique to Structural Analysis of Self-assembled Structures Consisting of Peptide Foldamers

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A well-designed beta-peptide foldamer can self-assemble to create various well-defined 3D architectures in aqueous solutions. The term foldecture is combination of the words foldamer and architecture. Our group has reported several unprecedented shapes of foldectures, such as a windmill and a molar tooth. These were highly homogenous both in terms of their size and morphology. Furthermore, to explore their potential use as functional materials, we recently published a study in which a carboxyl group was exposed to specific rhombic facets of foldectures. We found new potential capabilities of foldecture in relation to their mechanical properties, such as an anisotropic shape of a micro-sized container through the creation of a hollow cavity inside the container. Meanwhile, research on the functionalization of foldectures is expanding, as comprehending the self-assembly process and the resulting 3D shapes requires additional work. Hence, the structural determination of the molecular packing structure of foldecture is essential. In relation to this, the powder X-ray diffraction technique has been utilized here due to the dimensions and kinetical experimental conditions of foldecture. A PXRD analysis with synchrotron radiation was adequate to determine the packing structure with well-organized bonds and angle restraints. Further, it was able to designate the absolute orientation of the foldamers involved based on the predicted preferred orientation approximation. The use of a PXRD analysis on foldecture aided the understanding of the shape and properties of the newly formed foldecture and can be expected to play a major role in designing original examples of foldecture in the future.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-2

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:10, Chair: Wonryeon Cho

Investigation of site-specific water dynamics inside PEMs using Overhauser Dynamic Nuclear Polarization Nuclear Magnetic Resonance

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Nuclear Magnetic Resonance (NMR) is widely used in many fields such as physics, chemistry, biology and medicine. It provides structural and dynamic information of matter through its non-destructive and chemically selective detection. Overhauser Dynamic Nuclear Polarization (ODNP) is the technic that enhances NMR signal using interaction between electron spins and nuclear spins and signals can be amplified to about order of 10 to 100 times[1]. To apply ODNP in non-magnetic materials, spin labels are positioned to specific points of samples as a donor of electron spins. ODNP technic uses dipolar interaction between electron spins and nuclear spins and it is possible to selectively enhance and observe NMR signals near the site of spin labels with 1-nm spatial resolution and the enhancement effect of ODNP is related to the relative mobility of nuclear bearing particles and electron spins. Therefore, ODNP enables to observe local dynamics of particles near spin labels inside samples[2]. We have constructed X-band ODNP-NMR system by modifying an EPR spectrometer and an NMR spectrometer. Using this system, water dynamics inside Nafion was investigated as a function of concentration of various spin labels.[1] J. M. Franck et al. *Prog. in NMR Spectroscopy* 74 33-56 (2013)[2] B. D. Armstrong and S. Han *The Jour. of Chem. Phys.* 127 104508 (2007)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-3

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:20, Chair: Wonryeon Cho

A colorimetric probe to determine NO₂⁻ using label free gold nanocrystals

Kyungmin Kim, Yun Sik Nam¹, Kang-Bong Lee^{2,*}

Department of Chemistry, Korea University, Korea

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

²*Green City Technology Institute, Korea Institute of Science and Technology, Korea*

A simple and sensitive colorimetric method for the determination of NO₂⁻ ions in aqueous samples was developed using gold nanocrystals (AuNCs). The NO₂⁻ ion is selectively etched AuNCs and changing the particle shape. This etching resulted in a dramatic color change from vivid blue to light red. Using this methodology, the concentration of NO₂⁻ ions in environmental, biological and sitological samples could be quantitatively detected by the naked eye or by using UV-Vis spectrometry. Also, we found that the selectivity and sensitivity of the detection was noticeably improved at the 20mM of NaCl concentration, at which a more obvious color change was observed. The absorption ratios (A₅₅₀/A₆₅₀) of the modified AuNCs solution exhibited a linear correlation with NO₂⁻ ion concentrations within the linear range of 0.0~10 ppm, and the limits of detection in tap water, pond water and waste water were 38.45 nM and 0.46 μM, respectively. This cost-effective sensing system allows for the rapid and facile determination of NO₂⁻ ions in aqueous samples.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-4

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:22, Chair: Wonryeon Cho

Analysis of Correlation between Structure of Linear Surfactants and Acute Eye Irritation Scores

Sujin Cho, Tian Tian, Seog Woo Rhee *

Department of Chemistry, Kongju National University, Korea

In this work, we determined the eye irritation scores of surfactants with linear alkyl chains by HET-CAM assay using hen's eggs and investigated the correlation between the structure of surfactants and eye irritation scores. Surfactants with a cationic (ammonium salt), neutral, anionic (sulfate) head groups and a linear alkyl chain with 8 to 16 carbons as the tail group were selected. The properties of surfactant forming micelles in aqueous solution were measured by an electrical conductivity method and an absorbance measurement method. The eye irritation scores of surfactants at various concentrations were measured by the HET-CAM assay using hen's eggs as an alternative animal test. Based on the experimental results, we found a significant correlation between the structural properties of the surfactant and the critical micelle concentration, and the acute irritation score of the surfactant. The results of this study will be used to develop cell-based devices using microfluidic chips that can replace the HET-CAM assay.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-5

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:24, Chair: Wonryeon Cho

Assessment of Phototoxicity Inhibition of Flavone-based Materials

Sung Eun Lee, Tian Tian, Seog Woo Rhee*

Department of Chemistry, Kongju National University, Korea

In this work, we investigated the phototoxicity inhibition process of flavone-based materials using the 3T3 NRU assay, an in vivo acute phototoxicity evaluation method. Amiodarone HCl and chlorpromazine HCl were used as phototoxic materials, and chrysin and apigenin were used as photoinhibition inhibitors. The phototoxicity index, PIF value and MPE value, were calculated based on the cell viability measured as a function of concentration. When cells were treated with solutions containing both chlorpromazine and flavone-based materials, both chrysin and apigenin reduced the phototoxicity of chlorpromazine by UVA. In addition, we will discuss the cytotoxic and phototoxic mechanisms of each material and the phototoxicity inhibition process of flavone-based materials.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-6

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:26, Chair: Wonryeon Cho

Sequential colorimetric detection technology of iron and mercury ions by etching and aggregation of gold nanorods

Sujin Yoon, Yun Sik Nam, Kang-Bong Lee^{1,*}

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¹*Green City Technology Institute, Korea Institute of Science and Technology, Korea*

A simple and sensitive colorimetric assay method for the sequential determination of iron ions and mercury in aqueous samples was developed using label free gold nanorods. Iron ions etched gold nanorods, and mercury ions bond these gold nanorods together. This sequential react results in a dramatic color change from red to blue and finally back to red. Therefore, the concentration of iron ions and mercury ions in environmental samples can be quantitatively detected by the naked eye or by UV-Vis spectrometry when using the AuNRs sensor. The sensitivity of the detection is significantly improved by modulating the solution to pH 7, leading to a more rapid color change in the optimized AuNRs system. The absorption ratios (A_{640}/A_{740}) of the modified AuNRs solution exhibited a linear correlation with the iron ion concentrations. The absorption ratios (A_{550}/A_{640}) of the modified AuNRs solution exhibited a linear correlation with the mercury ion concentrations, with a limit of detection of 25.2 nM. This cost-effective detection system allows for the rapid and facile determination of the concentration of iron ions and mercury ions in aqueous samples.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-7

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:28, Chair: Wonryeon Cho

Morphological elucidation of porous PCL(Polycaprolactone) microsphere using various analytical methods

SUK YEN KO, Wangsoo Shin^{1,*}, Jinsu Kim¹, NAJEONG PARK¹

Analytical Science Center, R&D center, Korea

¹*MD program, R&D center, Korea*

The surface and internal morphology of biodegradable PCL(Polycaprolactone) microsphere was investigated in order to understand how can the porosity be distributed. The PCL microsphere were manufactured for medical use. The size distribution was measured by electrical sensing zone type particle size analyzer. And the surface porosity was observed using SEM. For the inner pore observation, first we confirmed that there were inner pores in the microsphere by OM. But PCL's low melting point of around 60°C and a glass transition temperature of about -60°C made it difficult to observe the cross-sectional image of the inner pore. It means that the conventional technique such as Microtome and cryo-CP methods were not available for PCL microsphere cross-section image and inner pore evaluation. We applied some ideas for solving this problem. Total porosity of PCL microsphere was measured using Mercury Porosimeter. Then we recalled the Mercury intruded samples and made cross-sectional cuts easily in the LN2 environment thanks to the occupied Mercury volume. The inner and under surface pore was observed using EDS mapping Mercury image. The micro-CT technique was not applicable in this study because of the mismatching spatial resolution.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-8

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:30, Chair: Wonryeon Cho

Effect of Adsorbate Molecules on Chemical Interface Damping in Single Gold Bipyramids with Sharp Tips

SOYOUNG LEE, JI WON HA*

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Single metallic nanoparticles are gaining much attention as an attractive biomolecular sensor. Especially, gold bipyramids (AuBPs) are expected to be a promising material for biosensors to have high detection sensitivity due to its sharper tips compared with spherical gold nanoparticle or rod-shape gold nanoparticle. They have higher sensitivity to refractive index of attached target molecules than spherical gold nanoparticles and gold nanorods. However, the conventional localized surface plasmon resonance (LSPR) sensing mechanism is affected by both the change of dielectric medium constant and the chemical adsorption onto the nanoparticle surface. Herein, we performed single particle spectroscopic study to characterize the effect of the medium dielectric constant and chemical binding of various thiol molecules on the LSPR linewidth in single AuBPs. More specifically, we demonstrate how chemical binding of various adsorbate molecules affects the LSPR linewidth of the longitudinal surface plasmon of single AuBPs. We found that the LSPR linewidth of single AuBPs remains almost constant when varying the refractive index of surrounding medium. However, thiol binding resulted in the redshift and broadening of LSPR spectrum of single AuBPs. Therefore, the results suggest that chemical interface damping of single AuBPs can be used to develop a LSPR biosensor that is only sensitively to the adsorption of biomolecules without interference from the dielectric constant of the surrounding medium.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-9

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:32, Chair: Wonryeon Cho

Decontamination of sulfur mustard in sand, concrete, and asphalt matrices

Hyunsook Jung

CBR Division, Agency for Defense Development, Korea

The persistence of sulfur mustard is still a major challenge for decontamination, as it remains in the environment after longer intervals of time. Decontamination involves multiple mass transport mechanisms, such as diffusion and chemical interactions among a contaminant, a decontaminant, and material interfaces. The complex series of interacting processes can contribute to post-decontamination hazards, such as vapor emission and contact transfer to humans and the environment. The present work is concerned with the decontamination of sulfur mustard on sand, concrete, and asphalt. This array of matrices was chosen to represent complex surfaces commonly observed in an urban environment that would be expected to be easily targeted by terrorists or rogue organizations. The results show that the whole amount of the mustard agent was not decontaminated, and 2 ~ 3 % of the preliminary quantity remained after the decontamination process, which was emitted as vapor over time. Not only vapors of the residual agent but also its byproducts, including sulfoxide and sulfone compounds, were gradually emitted from the decontaminated surface over time. For such byproducts, the hypochlorite ion (OCl^-), an active ingredient in the decontaminant used, reacts with sulfur mustard by oxidation to sulfoxide and/or sulfone and by dehydrochlorination to form such compounds as divinyl sulfone, which are reported to be relatively nontoxic.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-10

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:34, Chair: Wonryeon Cho

Surface-Enhanced Raman Scattering of Gold Nanourchins with Sharp and Short Branches

MINJUNG SEO, JI WON HA*

Department of Chemistry, University of Ulsan, Korea

Raman spectroscopy is a useful technique to observe vibrational, rotational, and other low-frequency modes in a system. Raman spectroscopy is complementary with IR and can be used when IR is forbidden. But, spontaneous Raman scattering is typically very weak compared with Rayleigh scattering because Raman intensity is almost 0.001% of the source intensity. Therefore, it is important to develop methods to enhance the signals. SERS (Surface Enhanced-Raman Scattering) is one of the methods that can enhance the signals up to 10^{11} . It is the basic principle of SERS that enhances Raman scattering by molecules adsorbed on rough metal surfaces or nanostructures. Various conditions are required for SERS. In the present study, we tried to optimize SERS with gold nanourchins (AuNUs) having sharp tips and rough surface. We tried SERS effect with R6G, p-aminothiophenol as probe molecules, 100-nm AuNUs. Raman spectra were measured with confocal homemade-Raman spectroscopy, and a 785-nm diode laser was used as a radiation source. LSPR peak of 100-nm AuNUs is close to 785-nm laser for resonance effect.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL1.O-11**

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:36, Chair: Wonryeon Cho

Defocused Dark-Field Orientation Imaging of Single Gold Microrods on Synthetic Membranes

Junho Lee, JI WON HA*

Department of Chemistry, University of Ulsan, Korea

Plasmonic gold microrods (AuMRs) are promising optical probes because of direct observation of their in-plane orientations and motions under an optical microscope. However, our understanding on the optical properties of AuMRs is still very limited at the single particle level and their out-of-plane orientations cannot be resolved by eye with high accuracy. Herein, we present the scattering properties of 1 μm -long AuMRs under defocused DF microscopy. Characteristic defocused scattering patterns of single AuMRs allowed us to resolve both in-plane and out-of-plane angles of single AuMRs. We further demonstrate the feasibility of using the defocused orientation imaging technique to track rotational motions and out-of-plane angles of single AuMRs on synthetic membranes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-12

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:38, Chair: Wonryeon Cho

Label-free Optical Biosensor Based on Chemical Interface Damping Using Gold-nanorods

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We studied the optical properties of gold nanorods using a darkfield microscope(DF) and a scanning electron microscope(SEM). The existing LSPR based biosensor was a method of sensing by the shift of the SPR peak when the target molecule was attached. However, the dielectric constant of the surrounding medium affects this sensing method. So, we propose a label-free plasmon-based biosensor that is sensitive to the adsorption of biomolecules without being disturbed by the dielectric constant of the surrounding medium. When thiol is attached to gold nanorods, wavelength shifts and FWHM (Full Width at Half Maximum) are increase. This is called chemical interface damping(CID). As the line width increases, sensing becomes possible without being affected by the dielectric constant. We propose a biosensing method based on CID by confirming the change of the optical characteristics according to the aspect ratio and the broadening of the plasmon line width of the rod-shaped gold nanoparticles by using three kinds of gold nanorods having different aspect ratios.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-13

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:40, Chair: Wonryeon Cho

Effect of Adsorbate Electrophilicity and Spiky Uneven Surfaces on Single Gold Nanourchin-based Localized Surface Plasmon Resonance Sensors

geunwan kim, JI WON HA *

Department of Chemistry, University of Ulsan, Korea

We present single particle studies on urchin-shaped gold nanoparticles for their use as localized surface plasmon resonance (LSPR) biosensors under dark-field (DF) microscopy. First, the LSPR wavelength of single gold nanourchins (AuNUs) was red-shifted as thiol molecules were attached onto the surface. AuNUs with sharp tips showed higher sensitivity for detecting thiol molecules than gold nanospheres (AuNSs) of similar size. Second, the degree of red shift was strongly affected by the electrophilicity of adsorbate molecules on the nanoparticle surface. Single AuNUs capped with 4-nitrothiophenol (4-NTP) strong electron withdrawing groups (EWG) caused a larger red shift than those coated with 4-aminothiophenol (4-ATP) strong electron donating groups (EDG). Last, real-time monitoring of molecular binding events on single AuNUs was performed. The LSPR peak was red-shifted and saturated after introducing 1 μ M of 4-aminothiophenol. Therefore, single AuNUs were highly sensitive to changes in medium dielectric constant as well as the electrophilicity of attached thiol molecules. The results indicate that single AuNUs with sharp tips can be used to develop highly sensitive LSPR biosensors.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-14

Area: Oral Presentation of Young Analytical Chemists I

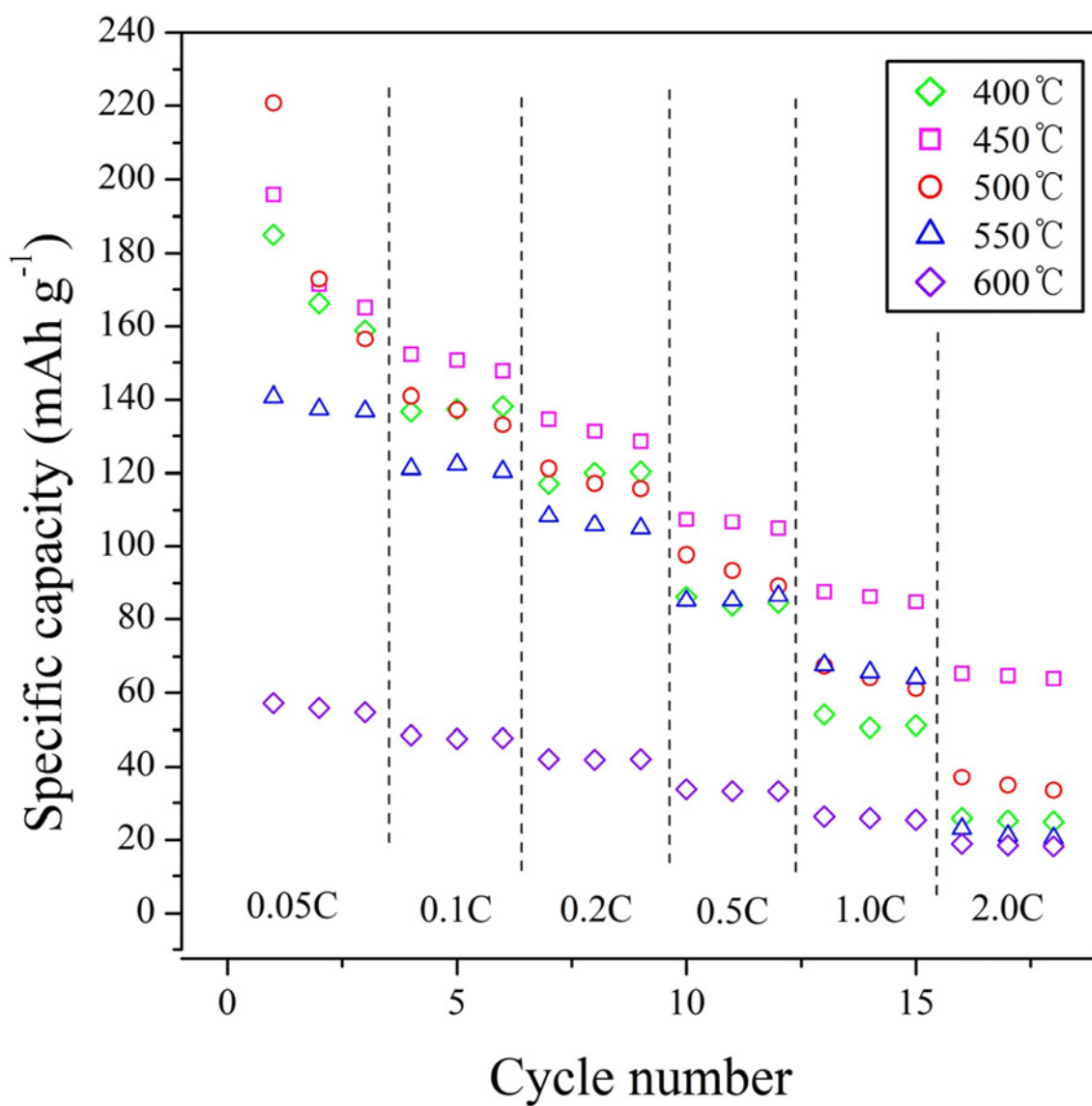
Type: Oral Presentation, Time: THU 09:42, Chair: Wonryeon Cho

Synthesis and characterization of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ cathode material prepared by a citric acid based sol-gel route

Minsoo Ji, YOUNGIL LEE*

Department of Chemistry, University of Ulsan, Korea

A new cathode material, $\text{Li}_3\text{V}_2(\text{BO}_3)_3$, has been calcined by citric acid based sol-gel route at various temperatures ranging from 400 °C to 600 °C and characterized for optimization of calcination temperature. The $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ as cathode material for LIBs was investigated on electrochemical performances. Citric acid acts not only as a chelating agent but also as a carbon source, which enhance the conductivity of the composite material and hinder the growth of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ particles during preparation. The structure and morphology of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ were characterized by X-ray diffractometry (XRD) and scanning electron microscopy (SEM). Galvano-static charge/discharge and cyclic voltammetry (CV) measurements were used to study its electrochemical behaviors which indicate the reversibility of the lithium extraction/insertion processes. The sample synthesized at 450 °C exhibits the highest capacity of 198 mAh g⁻¹ at 0.05C and excellent cycle ability.



AMERICAN CHEMICAL SOCIETY

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-15

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:44, Chair: Wonryeon Cho

Study of electrochemical properties for porous $\text{Li}_3\text{V}_2(\text{BO}_3)_3/\text{C}$ as a cathode material its characterization using MAS NMR for Li-ion batteries

Ji Won Lee, CHAEWON Moon, YOUNGIL LEE*

Department of Chemistry, University of Ulsan, Korea

Recently, poly-anion based compounds such as phosphates, silicates and borates as cathode materials for Li-ion battery have been developed for using in individual IT device, electric vehicles, and high energy storage systems have been investigated due to low cost and structural stability. Among these compounds, monoclinic $\text{Li}_3\text{V}_2(\text{PO}_4)_3/\text{C}$ (LVP) has good thermal stability, structure stability and the highest theoretical specific capacity of 197 mAh g^{-1} in the potential range of 3.0 – 4.8 V. However, LVP has low electronic conductivity and Li-ion diffusion coefficient (10^{-8} to $10^{-14} \text{ cm}^2 \text{ s}^{-1}$). So, we have attempted to fully exchange the phosphate to the borate in order to improve specific discharge capacity. This material has been synthesized by combustion synthesis method and the morphology, compositions and electrochemical performance of the synthesized sample were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Cycling test and Galvanostatic charge-discharge measurement and mainly analyzed the structure character using solid-state MAS NMR. As a result, we demonstrates the electrochemical performances of a highly porous $\text{Li}_3\text{V}_2(\text{BO}_3)_3/\text{C}$, synthesized via combustion synthesis as a new cathode material with a wide range voltage operability of 0.9 to 4.5 V which delivered exceptionally high discharge capacity 257 mAhg^{-1} at 0.05 C, 95.6% of its theoretical capacity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-16

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:46, Chair: Wonryeon Cho

Chromatographic Enantiomer Separation of Chiral Amines as Nitrobenzoxadiazole Derivatives on Several Polysaccharide-Derived Chiral Stationary Phases by Normal HPLC under Simultaneous Ultraviolet and Fluorescence Detection

Adhikari Suraj, Wonjae Lee*

College of Pharmacy, Chosun University, Korea

A convenient and derivatized method using a fluorogenic agent, 4-chloro-7-nitro-1,2,3-benzoxadiazole (NBD-Cl) was developed for enantiomer resolution of chiral aliphatic amines including amino alcohols by normal HPLC. The enantiomer separation of chiral amines as NBD derivatives was performed on six covalently bonded and four coated type polysaccharide-derived chiral stationary phases (CSPs) under simultaneous ultraviolet (UV) and fluorescence detection (FLD). Among the covalently bonded CSPs, Chiralpak IE showed the best enantiomer separation for most analytes. The other CSPs also showed good enantioselectivity except for Chiralpak IB. On the other hand, Chiralpak AD-H and Amylose-1 generally exhibited better enantiomer separation of NBD derivatized chiral amines among the coated CSPs. The developed analytical technique was also applied to determine the optical purity of commercially available (R)- and (S)-leucinol; the impurity was found to be 0.06%. The developed method was validated and proved to be an accurate, precise, sensitive and selective method suitable for enantiomer separation of chiral aliphatic amines as NBD derivatives under simultaneous UV and fluorescence detection.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-17

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:48, Chair: Wonryeon Cho

Forensic Platform for Identification of Human Saliva using MS-based Glycomics

Hantaek Moon, Bum Jin Kim, Hyun Joo An*

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

In forensics, saliva found at crime scenes is one of the important evidences and thus, the identification of human saliva from other human fluids and non-human fluids, respectively is an essential prerequisite prior to further crime investigation. In previous study, we could determine that the degree and amount of highly fucosylated N-glycans were specific features to identify human saliva from other body fluids through MS-based glycomic approach. However, most saliva encountered at crime scenes has a trace amount and has been often found as a dry spot. For these reasons, forensic platform with high sensitivity for identification of human saliva is required. Herein, we have developed MS-based platform using glycomics and characterized N-glycans extracted from a trace amount of dried saliva. Briefly, dried saliva was prepared by spotting the saliva onto a protein saver card and drying at ambient temperature. N-glycans were enzymatically released by PNGase F from dried saliva spot (DSS) and enriched by solid phase extraction with a porous graphitized carbon cartridge. Then, saliva N-glycans were characterized by MALDI-TOF/TOF MS. N-glycans found in DSS showed a high correlation in terms of the number of glycans and their amount compared with N-glycans released from saliva fluid. Indeed, highly fucosylated N-glycans were also observed as a specific signature in DSS. We also examined technical validated reproducibility of N-glycan analysis based on DSS. This is the first study to apply a glycomic tool to forensic science.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-18

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:50, Chair: Wonryeon Cho

High-throughput Automated Platform for Native Glycan Analysis using Liquid Handling System

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Glycosylation of therapeutic glycoproteins is a key factor influencing biological function, safety, and protein stability. To assure quality of biopharmaceuticals, glycosylation should be analyzed at all stages of manufacturing process since it could be changed by cell culture and environmental conditions. For sample preparation, automated system is often necessary in pharmaceutical industry to reduce hands-on time and to obtain accurate and reproducible data. Here, we present the robotic platform to release and enrich glycans from glycoproteins by liquid handling system combined with 96-well microplate. Overall processes including protein denaturation by heating block, N-glycan release by PNGase F, and glycan enrichment by solid phase extraction (SPE) were automatically performed. Especially, the technical variation was mostly affected by PGC-SPE to purify and fractionate different types of glycans. For setting up SPE conditions, we used glycoprotein mixtures including diverse glycans which were eluted by varying proportions of acetonitrile in water and formic acid. Consequently, we obtained three eluents consisting of high-mannose and complex-type glycans w/wo sialic acid residues. Automated full steps for glycan preparation is being repeatedly performed to validate the technical reproducibility of our platform. Ultimately, it can be applied for monitoring bioactive glycans of biotherapeutics or clinical glycan biomarkers.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-19

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:52, Chair: Wonryeon Cho

Molecular level characterization of chemical compounds in crude oil deposit from tanks in Artawi oil field (Iraq)

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Molecular level characterization to identify and measure the deposits from the petroleum fluids were performed. The crude oil deposit was obtained from tanks located at Artawi field in south of Iraq /Basrah. Separation by centrifuge and filtration were used to prepare the sample. The samples were fractionated into three layers (upper part deposit sticky, middle part water and lower part deposit soil). The chemical compounds in the crude oil deposit were characterized by using ultra-high resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) along with (+) mode atmospheric photoionization (APPI) and (-) mode Electrospray Ionization (ESI) ion source. FT-ICR MS analysis provides comprehensive heteroatoms class distribution. The deposit of crude oils yielded distributions of hydrocarbons and heteroatoms. The results of such analysis showed the hydrocarbons are more abundant in the oil deposit soil, while the crude oil and deposit of crude oil sticky showed the heteroatoms are more abundant than hydrocarbons. Therefore, these procedures provide an understanding of the overall behavior of the species that precipitate as well as of the interactions among those compounds.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-20

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:54, Chair: Wonryeon Cho

Quantification of Inorganic Arsenic using Ion Exchange Membrane by Laser Induced Breakdown Spectroscopy

Kwon seul woo, Sang-Ho Nam^{*}, Yonghoon Lee

Department of Chemistry, Mokpo National University, Korea

The toxicity, bioactivity and mobility of arsenic are dependent on the chemical forms or species in which it exists. It is well known that the inorganic arsenic is more toxic than the organic arsenic. Inductively Coupled Plasma-Mass Spectrometry(ICP-MS) coupled with chromatographic technique has been used to perform the qualitative and quantitative determination of the arsenic species in various samples. However, it has been difficult to conduct a overall analysis due to matrix effects and took a long time to separate the arsenic species in various samples with the complex matrix. In this study, the solid phase extraction(SPE) membrane was used to separate inorganic arsenics, and those were detected by laser induced breakdown spectroscopy (LIBS). The samples were prepared using a buffer solution with phosphate buffer saline (pH 7.4) to separate arsenic species. The recovery efficiency of As(V) by LIBS was 96.9 %. NIST water CRM 1643f was used to validate the method for the determination of inorganic arsenics in a sample. The recoveries of As(V) and As(III) by LIBS were 98.9 % and 102.0 % respectively. The new speciation method by LIBS has labor and cost advantages for the quantitation of inorganic arsenic.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-21

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:56, Chair: Wonryeon Cho

Synthesis, dispersion and tribological potential of alkyl functionalized graphene oxide for oil-based lubricant additives

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Graphene has been reported as an excellent lubricant additive for reducing adhesion and friction when coated on various surfaces as an atomically thin material with low surface energy. We have developed graphene oxide (GO) grafted with long alkyl chains to improve dispersion in oil-base lubricant as largely enhanced lipophilicity. Alkyl functionalized GO is synthesized by reacting NH₂-GO with alkylchloride (n=4, 8, 14) in ethanol under reflux, then 0.02 wt% of alkyl functionalized GO (FGO 4, 8, 14) are added into the base oil (PAG 0W40) and ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene are investigated by Fourier transform infrared (FT-IR), X-ray photoelectron spectroscopy (XPS) and scanning electron microscope (SEM), Transmission electron microscopy (TEM), X-ray Diffraction (XRD) and Raman spectroscopy. The tribological tests are performed with High frequency friction/wear Tester. The van der Waals interaction between the tetradecyl chains grafted on GO and the alkyl chains of base oil provided long-term dispersion stability so that the C14-GO showed better dispersion than C4-GO, C8-GO. The C14-GO also decreased both friction and wear considerably under the rubbing contacts between ball and disk.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-22

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 09:58, Chair: Wonryeon Cho

Characteristics and electrochemical performance of silica coated carbon nanocoils composite as an anode material for lithium secondary batteries

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We have performed a study of a silica/carbon nanocoils (SiO₂-CNC) nanocomposite as a potentially high performance anode for rechargeable lithium secondary batteries. Carbon nanocoils were grown via chemical vapor deposition (CVD) method. Acetylene (C₂H₂) and Sulfur hexafluoride (SF₆) were flowed into the quartz reactor of a tubular furnace heated to 550 °C at 100 torr and maintained for 60 min to synthesize CNCs. CNCs were then put into the Tetraethyl orthosilicate (TEOS) to synthesize SiO₂-CNCs composite. The electrochemical characteristics of SiO₂-CNCs composites as an anode of Li secondary batteries were investigated using three-electrode cell. The SiO₂-CNCs composites loaded on Ni foam were directly employed as an working electrode without binder. As the counter and reference electrode used lithium foil. 1M LiClO₄ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC): ethylene carbonate (EC) in a 1:1 volume ratio. Glass fiber separator was used as the separator membrane. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. The morphologies, compositions and crystal quality of the prepared SiO₂-CNCs composites were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), energy X-ray diffraction (XRD), dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). As a result electrochemical performance of SiO₂-CNC was better than existing carbon nanofibers and carbon nanocoils.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-23

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:05, Chair: Wonryeon Cho

On-line proteolysis and glycopeptide enrichment using dual micro-scale porous polymer membrane enzyme reactor (μ PPMER) and nanoflow liquid chromatography-tandem mass spectrometry

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N-glycosylation is a type of glycosylation that occurs when glycans are attached to the nitrogen atom of asparagine (asn, N). It is important to analyze N-glycoproteins in biological samples as they play essential roles in protein folding or signaling process. However, analysis of glycoproteins from glycopeptides by shotgun analysis can be time-consuming and sample loss is inevitable during pre-treatments. Therefore, to overcome such problems, dual micro-scale thermo-sensitive porous polymer membrane enzyme reactors (μ PPMER) has been utilized for on-line proteolysis, followed by enrichment of glycopeptides prior to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS/MS). A thermo-responsive porous polymer membrane (T-PPM) was synthesized by coating PS-co-MAN-NIPAM polymer on bare nylon membrane and its characterization was conducted by SEM. Trypsin and lectin were immobilized on the coated membrane for proteolysis and glycopeptide capture, respectively, and each of membrane was inserted in μ PPMER module. Dual μ PPMER modules were connected to nLC-ESI-MS/MS system for on-line analysis and efficiency in glycopeptides enrichment selectivity under various temperatures were evaluated. In addition, glycoproteins from human plasma and urine samples were analyzed using on-line dual PPMER module in the most optimized condition for glycopeptide enrichment.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-24

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:07, Chair: Wonryeon Cho

Effect of high fat diet on mouse brain lipidomes by nUPLC-ESI-MS/MS : Cortex, Hippocampus, Hypothalamus, & Olfactory bulb

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Lipids are known to be involved in various neuronal functions in brain, which is one of the most important and complex organ in the central nervous system. As brain plays a number of roles including cognition, memory, learning, and metabolic control, brain dysfunction can eventually lead to a variety of diseases. Recently, lipidomic analysis in relation to brain diseases has attracted much attention. High fat diet (HFD) can cause insulin resistance in the brain tissues by inducing obesity through diet. Although the effects of HFD on brain health have been studied in pathology, the relationship between HFD and brain lipid profiles has not been extensively studied. In this study, four different brain tissues (cortex, hippocampus, hypothalamus, and olfactory bulb) from mouse upon high fat diet programs have been analyzed using nanoflow ultrahigh pressure LC-ESI-MS/MS (nUPLC-ESI-MS/MS) for the investigation of HFD effect on the changes in the lipid profiles. Mice were fed with the various dietary plans: 8 weeks normal control (N), and weight gain (F), 16 weeks normal control (NNN), weight maintenance (FNN), weight gain (NNF), and weight cycling (FNF). As a result, 270 lipids including phospholipid, glycerolipid, and sphingolipid were quantified and statistical analysis was applied.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-25

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:09, Chair: Wonryeon Cho

Analysis of HDL from coronary artery disease patients through bottom-up and top-down proteomic approach using flow field-flow fractionation and mass spectrometry

Jae-Hyun Lee, JoonSeon Yang, Myeong Hee Moon*

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Coronary artery diseases (CAD) is a disease caused by narrowing of the coronary arteries of the heart by plaque, fat or other substances. Narrow coronary artery interfere with blood flow to heart and may even cause damage in heart or eventually lead to death. High-density lipoprotein (HDL) has been reported to be associated with CAD as marker molecules. Lipoprotein is known as a macromolecules that transports lipids through the blood. These lipoproteins are divided into different classes depending on their density and specific role. HDL is composed of lipid and various proteins including apolipoproteins. One of the roles of HDL to transport excess cholesterol to the liver and regulate cholesterol levels in cells, blood vessels, and blood. Transportation of cholesterol by HDL helps to remove excessive cholesterol out of cells, blood, and blood vessel wall. Recent studies have been reported that apolipoprotein A-I in HDL goes through oxidation in severity of CAD. Flow field-flow fractionation (FIFFF) is widely used to separate macromolecules and nanoparticles according to their hydrodynamic diameter. In this study, HDL from human plasma of CAD patients was separated by FIFFF. Miniaturized asymmetrical FIFFF (AF4) channel was coupled on-line to electrospray ionization mass spectrometry (ESI-MS) for a high speed separation of lipoproteins and top-down proteomic analysis for various proteins including ApoA-1 from HDL were analyzed in order to investigate the change in HDL-related proteins caused by severity of CAD.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-26

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:11, Chair: Wonryeon Cho

Steric Transition Phenomena upon Field Decay Patterns Using Frit-inlet Asymmetrical Flow Field-Flow Fractionation

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Flow field-flow fractionation (FIFFF) is a separation technique that can separate macromolecules by size without stationary phase. The separation mode of FIFFF can be divided into normal and steric/hyperlayer mode; particles with sizes smaller than 1 μ m are operated in normal mode while those larger 1 μ m are operated in steric/hyperlayer mode. During the focusing/relaxation process, smaller particles diffuse more and equilibrate at a position higher from the channel than larger particles. As a result, The smaller particles are located in faster flow stream and eluted earlier than the larger particles. In the steric/hyperlayer mode, where the particle size is larger than 1 μ m, Brownian diffusion becomes negligible and particles are elevated to a certain height by lift force. Since the larger particles have higher lift forces than the smaller particles, they elute earlier. Steric transition is a phenomenon that particle elutes by a combination of normal mode and steric mode in FIFFF. Frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) operates by stopless flow without focusing process. In this study, steric transition phenomenon is systematically monitored with polystyrene particles by FI-AF4 coupled with UV/visible detector and multi-angle light scattering. Depending on the strength and gradient of the field, the particle size at which the steric transition occurs varies. Therefore, it is possible to increase the range of particle size separated in the normal mode.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-27

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:13, Chair: Wonryeon Cho

Profiling of lipoproteins from patients with mild cognition impairment and Alzheimer's disease by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

SAN HA KIM, JoonSeon Yang, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Recently, as the average life span of people is increasing, the number of elderly population has been rising sharply and cognitive impairment disorders with aging factor such as Alzheimer's disease have become common. Amyloid-beta plaques is known to be a major cause of Alzheimer's disease and kills neighboring brain cells, which leads to dysfunction in cognitive abilities. Symptoms of Alzheimer's disease's are usually developed decades after the accumulation of amyloid-beta. Therefore, the rate of disease progression is even faster when symptoms start to appear. About 10 percent of patients with mild cognitive impairment, a pre-stage of Alzheimer's disease, end up diagnosed with Alzheimer's disease within a year. Several studies have reported that high levels of low-density lipoprotein(LDL) and low levels of high-density lipoprotein(HDL) is affected amyloid-beta. Therefore, it is important to understand lipid metabolism from separating HDL and LDL, separately. In this study, lipids from human plasma samples of healthy controls, patients with mild cognition impairment, and Alzheimer's disease patients were analyzed. Lipoproteins were fractionated by asymmetrical flow-field flow fractionation and the lipids were extracted from the collected fractions of HDL and LDL and structurally identified from collision-induced dissociation of nanoflow ultrahigh-pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS). More than 300 lipids were identified. Identified lipids are quantified from individual samples to evaluate the difference between the two groups in comparison to those of healthy controls.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-28

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:15, Chair: Wonryeon Cho

Lipidomic analysis of blood plasma from patients among five different cancer types by nUPLC-ESI-MS/MS

Gwang Bin Lee, JongCheol Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

As lipids are associated with functions such as chemical-energy storage, cellular signaling, cell membranes, and cell to cell interaction, they play a key role in cellular survival, proliferation, and death. These cellular processes are vitally concerned with carcinogenesis pathways, especially to transformation, progression, and metastasis, suggesting the bioactive lipids are mediators of a number of oncogenic processes. According to recent lipidomics research, lipid analysis regarding cancer is very important, since each type of cancer has different carcinogenesis pathways. In this study, lipids from plasma of healthy controls and patients with cancers (liver, stomach, lung, colorectal, and thyroid) were investigated in order to discover lipids that show significant difference between the groups and find potential lipid biomarkers for each cancer. Blood plasma were extracted from each control and cancer patients using the modified Folch method with MTBE/methanol, and the extracted lipids were analyzed by nLC-ESI-MS/MS. A total of 243, 236, 239, 239, and 225 lipids from plasma of patients with liver, stomach, lung, colorectal, thyroid cancer, and controls, respectively, were identified and profiling of lipid from each case of cancer was compared with that of controls.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-29

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:17, Chair: Wonryeon Cho

An investigation on the various internal standards for the accurate determination of the arsenic species in rice

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Rice is a staple food in the world's half population and is a major source of human arsenic intake. But, toxicity of arsenic depends on its chemical forms. Therefore, the selective and quantitative determination of the total arsenic as well as the arsenic species in rice has been very important. However, the extraction and determination of arsenic species in rice has been very difficult because of the severe matrix interference. In this study, the various analytical methods including the internal standard method and standard addition method have been investigated for the determination of arsenic species in rice. The extraction solvent has been used 0.28 M nitric acid. A new analytical method was developed for the determination of arsenic species in rice by inductively coupled plasma - mass spectrometry (ICP-MS) coupled with ion chromatography (IC). Rice certified reference material (NIST SRM 1568b rice flour) was used to evaluate its suitability for the analytical method. In this study, two internal standards were used. The first internal standard was injected before sample introduction to correct the signal change with time, and the second internal standard was spiked into the sample to remove or reduce the matrix interferences. Recoveries of inorganic arsenic, DMA, MMA, and total arsenic for the certified values were 92 %, 116 %, 107 % and 107 %, respectively, with the developed method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-30

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:19, Chair: Wonryeon Cho

LC-MS/MS determination and pharmacokinetic study of Sorafenib in rat and beagle plasma

yoojeong yoon

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A rapid, sensitive and selective liquid chromatography/tandem mass spectrometry method (LC-MS/MS) has been developed and validated for the identification and quantification of Sorafenib in rat and beagle plasma using Sorafenib-d3 as an internal standard. Sample pretreatment involved simple protein precipitation (PPT). Chromatographic separation was carried out on a poroshell 120 EC-C18 column (3.0 × 50mm, 2.7 μm, Agilent) at 35 °C using an isocratic elution method with acetonitrile/0.1% formic acid in 10mM ammonium formate: 70/30 (v/v) at a flow rate of 0.2mL/min. Detection was performed using electrospray ionization in positive ion multiple reaction monitoring (MRM) mode by monitoring the ion transitions from m/z 465.3 → 252.2 (Sorafenib) and m/z 468.1 → 255.0 (internal standard). Calibration curves were linear in the concentration range of 5–5000 ng/mL. The overall precision and accuracy for all concentrations of quality controls and standards were better than 15%. The validated method was successfully applied to the pharmacokinetic study of Sorafenib in rat and beagle plasma..

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-31

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:21, Chair: Wonryeon Cho

Synthesis and Characterization of Graphene-enfolded TiO₂ Anatase as Anode Materials for Li-Secondary Batteries

Hasan Jamal

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In this study, graphene-bonded and enfolded anatase TiO₂ of various types composites have been synthesized without using any cross-linking reagent, by using graphene oxide (GO) and titanium dioxide as a precursor. In which graphene sheets are uniformly dispersed among the TiO₂ anatase particles, in order to enhance the cyclic ability and electronic conductivity of TiO₂ anode for lithium ion batteries. The composites of GO with three types of anatase TiO₂ (Nanoparticles, Nanorods, Nanofibers) were synthesized by hydrothermal and calcination treatment. The reduction of GO was simultaneously proceeded after the calcination in an argon atmosphere at 400 °C for 4 h. The physicochemical properties were characterized by Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. Surface properties were measured by BET & BJH method. The electrochemical properties were also investigated by cyclic voltammetry (CV) and Electrochemical Impedance Spectra (EIS). The TiO₂ nanorods/graphene composite having unique morphology showed superior discharge capacity of 135 mAh g⁻¹ at a current density of 0.5 C than other types of TiO₂ composites and achieved a reversible capacity of 105 mAh g⁻¹ after 35 cycles.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL1.O-32

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:23, Chair: Wonryeon Cho

Quantitative analysis of residual lactide in Polylactide by NMR and GC

HYERIM KIM

Samyang Biopharmaceuticals Corp., Analytical Science Center R&D Center, Korea

Poly(lactide)(PLA) is one of the biodegradable aliphatic polyesters and has been widely applicable in the field of bio-medicine and environmentally friendly products. Industrially, PLA is produced by ring-opening polymerization of lactide in bulk, and purified through de-volatilization at high temperature under high vacuum. The performances of PLA are directly affected by the content of residual monomer in polymers, such as having harmful effects during processing and also causing undesired property changes in the end products, lowering mechanical strength and thermal stability, and increasing the hydrolytic degradation rate of PLA products. In this study, We have developed methods to quantitatively determine the residual lactide monomer in PLA using NMR spectroscopy compared with conventional gas chromatography(GC) methods. There was no significant difference in the results of quantification of the residual lactide monomer in PLA by NMR and GC. So, NMR spectroscopy can be a powerful tool for the analysis of residual lactide.

120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL1.O-33**

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:25, Chair: Wonryeon Cho

[Withdrawal] Equipment for lung cancer diagnosis via breath analysis using IMS

HeeJin Moon

R&D, Sensor Tech, Korea



120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL1.O-34**

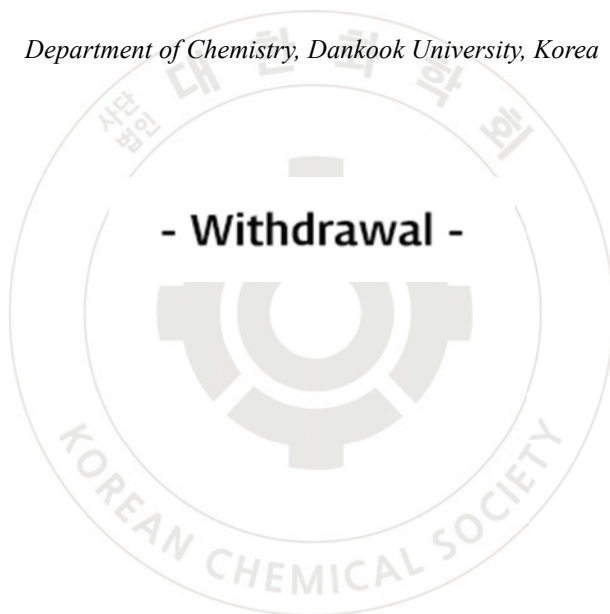
Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:27, Chair: Wonryeon Cho

**[Withdrawal] Study on boron analysis of NCM Anode active material
in lithium ion battery by ICP-MS**

In Gi Kim, Heung Bin Lim*

Department of Chemistry, Dankook University, Korea



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-35

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:29, Chair: Wonryeon Cho

Optimization of sample preparation for the identification of GB-tyrosine in rat plasma exposure to GB

JIHYUN KWON, Yong Gwan Byun, Yong Han Lee*

Agency for Defense Development, Korea

The identification of the chemical warfare agent, isopropyl methlyphosphonofluoridate (sarin, GB) in plasma has been studied using liquid chromatography-tandem mass spectrometry (LC-MS/MS). However, systematic study of sample preparation for LC-MS/MS was not done a lot. Therefore, the sample preparation for the identification of GB-tyrosine in rat plasma was studied. Also, the lowest detection concentration of GB-tyrosine for LC-MS/MS was reported using the optimized sample preparation. The optimized sample preparation will be employed to study other types of nerve agent in plasma.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL1.O-36**

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:31, Chair: Wonryeon Cho

Anti aging effect of green tea extract and its application to the herb material of emulsion base

Young Jun Park

Cha university, Korea

Jeju island is located at the south area of Korean peninsula. It has a natural resources of wild grown herbal medicine plants. Various species currently classified as herbs are grown or cultivated in Jeju. Recently, studies on catechin have attracted interest to control wrinkles aging on skin man and woman. The proposal of this study was to determine whether catechin compound mixture, the active ingredient, could be used as herbal extract to improve aging wrinkles, especially for middle aged group using various test. First, this study determined its elastase activity and anti oxidizing effect by DPPH assay in vitro, to evaluate the efficacy of emulsion catechin prototypes in improving anti aging. This study will provide basis for the development of catechin prototypes with advanced composition technology. It will add a step forward to the herbal cosmetic industry.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-37

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:33, Chair: Wonryeon Cho

Quantum Dot Dissolution Based Electrochemical Immunosensor for a Post Mortem Interval Biomarker Detection in Serum Sample

BongJin Jeong, RASHIDA AKTER, Jeonghyun Oh, Md. Aminur Rahman*

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

In the present work, an electrochemical post mortem interval biomarker immunosensor was fabricated on the and quantum dot (QD) attached graphene oxide (GO) incorporated cysteamine (Cys) self-assembled monolayer (SAM) based platform for the detection of glyceraldehyde 3-phosphate dehydrogenase (GAPDH) in human serum sample. Monoclonal anti-GAPDH antibody was covalently immobilized on the carboxylic acid functionalized cadmium selenide (CdSe) QD through the amide bond formation by EDC/NHS coupling. The immunosensor surface was characterized using scanning electron microscopy (SEM) and energy The GAPDH detection was made through the dissolution of the surface attached CdSe QD by glucose oxidase (GOx) enzyme generated hydrogen peroxide, which was used as an enzymatic label. For enhancing the sensitivity, we performed the competitive assay in which GD-GOx conjugates and free-GD competed for binding to the active sites of antibody. The current response resulted from the optimized CdSe dissolution was found to be decreased with increasing concentration of free GD and was proportional to the free-GD concentration. Differential pulse voltammetry (DPV) technique was used to determine the analytical characteristics such as detection limit (DL), linear dynamic range, selectivity, stability, and the real sample analysis for the GD detection. The proposed GAPDH immunosensor showed a wide linear range from 1.0 fg / mL to 100 ng / mL and exhibited a low detection limit of 2.0 fg / mL. The practical application of the immunosensor was tested in the human serum samples, which can be used in the forensic science field.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-38

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:35, Chair: Wonryeon Cho

Graphene Oxide/Polytyramine Nanocomposite Based Immunosensor for Electrochemical Protein Detection

MD. ARIF-UR RAHMAN, RASHIDA AKTER, BongJin Jeong, Jeonghyun Oh, Md. Aminur Rahman*

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The sensitive detection of a serum cytokine protein, interleukin-6 (IL-6) was carried out using a polytyramine/graphene oxide/ (Ptyr/GO) nanocomposite film based electrochemical immunosensor. Monoclonal anti-IL-6 antibody was covalently immobilized on the Ptyr/GO nanocomposite film through the covalent bond formation between the amine groups of Ptyr and antibody through the glutaraldehyde crosslinking. Magnetic bead (MB) supported numerous thionine (Th) labels were used for the sensitive detection of IL-6 through the electrocatalytic reduction of hydrogen peroxide (H₂O₂). The GO/Ptyr immunosensor surface was characterized using cyclic voltammetry (CV), scanning electron microscope (SEM), electrochemical quartz crystal microbalance (EQCM), and electrochemical impedance spectroscopy (EIS) techniques. Square wave voltammetric (SWV) technique was used to measure the electrochemical response after optimizing the experimental conditions. The proposed Ptyr/GO nanocomposite based immunosensor with MB-supported Th labels showed a low limit of detection (LOD) of 0.1 pg/mL and wide linear range between 0.5 and 100 pg/mL with excellent stability and enhanced selectivity. The detection ability of the proposed immunosensor was compared with an enzyme-linked immunosorbent assay (ELISA) method and was applied to various IL-6 spiked human serum samples.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-39

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:37, Chair: Wonryeon Cho

Improving Electrochemical Protein Detection through Enhancing Biocatalyzed Precipitation Using Bienzymes Coated Carbon Nanotubes

RASHIDA AKTER, MD. ARIF-UR RAHMAN, Jeonghyun Oh, BongJin Jeong, Md. Aminur Rahman *

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A highly sensitive electrochemical detection of mucin 16 (MUC16) based on enhanced biocatalyzed precipitations using bienzymes glucose oxidase (GOx) and horseradish peroxidase (HRP) coated multiwall carbon nanotubes (MWCNTs) was developed for the early diagnosis of ovarian cancer. The immunosensor was fabricated by covalently immobilizing monoclonal anti-MUC16 antibody on noncovalent functionalized graphene oxide (NGO) on gold nanoparticles (AuNPs) modified indium tin oxide (ITO) electrode (immunosensor probe). The MUC16 (target protein) and anti-MUC16/MWCNTs/GOx/HRP conjugate were bonded with the immunosensor probe through the immunoreaction. The biocatalyzed precipitation of 4-chloro-1-naphthol (CN) by bienzymes was then carried out at the immunosensor probe. The insoluble precipitates accumulated on the immunosensor probe and acted as a barrier for the direct electron transfer (ET) reaction of an external $\text{Fe}(\text{CN})_6^{3-}/\text{Fe}(\text{CN})_6^{4-}$ redox couple. The amplified detection was achieved through the increased ET blocking ability of the immunosensor by numerous precipitates using enormous numbers of GOx and HRP on MWCNT and the in situ generation of an enzymatic substrate, hydrogen peroxide (H_2O_2). The immunosensor surface was characterized using scanning electron microscope (SEM), quartz crystal microbalance (QCM), and electrochemical impedance spectroscopy (EIS) techniques. Cyclic and square wave voltammetric techniques were used to monitor the electrochemical responses before and after precipitation reaction. Under the optimized experimental condition, the proposed immunosensor with bienzymatic label showed a low limit of detection (LOD) and wide linear range, which were 10 times lower and wider than those obtained for an immunosensor with a single enzyme (HRP) label. The validity of the proposed method was compared with an enzyme-linked immunosorbent assay (ELISA) and was applied to various MUC16 spiked human serum samples for the selective detection of MUC16.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-40

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:39, Chair: Wonryeon Cho

Simultaneous Multiplexed Detection of Multiple Cancer Biomarkers using Graphene Oxide Electrode Array and Metal Ion Tagged Dendrimer Label

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The simultaneous multiplexed detections of three prostate cancer (PC) biomarkers, prostate specific antigen (PSA), prostate specific membrane antigen (PSMA), and interleukin-6 (IL-6) were carried out using a triple graphene oxide electrodes array on indium-tin oxide (ITO) and metal ion tagged dendrimer labels. To fabricate the immunosensor array, three monoclonal antibodies, anti-PSA, anti-PSMA, and anti-IL-6 were covalently immobilized on the three separate 1-pyrenecarboxylic acid (Py-COOH) functionalized GO modified ITO surface using EDC/NHS coupling. Three different types of metal ions such as Cu^{2+} , Cd^{2+} , and Zn^{2+} were coordinated with a third generation dendrimer with 32 surface terminated carboxylic acid groups through 5-aminoisophthalic acid, which were conjugated with three different types of antibodies. In the presence of the specific biomarker such as PSA, PSMA, and IL-6, the anti-PSA, anti-PSMA, and anti-IL-6 antibodies conjugated metal ions tagged dendrimer label attached to the immunosensor arrays. The multiplexed detection of three different types of biomarkers were achieved through directly monitoring the stripping current of the metal ions without any harsh acid dissolution step. Linear sweep voltammetric (LSV) technique was used to measure the stripping currents of respective metal ions in acetate buffer at pH 4.6 after optimizing the experimental conditions. The present immunosensor array exhibited low limit of detections (LODs) and wide linear ranges for three prostate cancer biomarkers with excellent stability and improved selectivity. The applicability of the proposed multiplexed immunosensor array was verified by comparing the immunosensor results with individual enzyme-linked immunosorbent assays (ELISA) for PSA, PSMA, and IL-6 was successfully tested to human serum samples for practical applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-41

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:41, Chair: Wonryeon Cho

Synthesis of Silicon-Coated Gold Nanoparticle for Dual Imaging and Therapy

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Gold nanoparticles (Au NPs) have been used as effective Surface-Enhanced Raman Spectroscopy (SERS) substrates for decades. We synthesized the Au NPs through seeded growth method using a sodium citrate as stabilizer and reducing agent. However, this citrate-stabilized Au NPs become unstable when the environment changes abruptly, and agglomeration and sedimentation usually occur because of the properties of the stabilizers on the Au NPs surface. Therefore, improving the stability of Au NPs has important significance. At present, there are many coating methods to stabilize the Au NPs, such as silver, alumina and so on. However, one such robust functionalization that has been proven to enhance gold nanoparticle stability both thermodynamically and chemically is silica coating. The synthesis of Au NPs and silica coating were confirmed by UV spectroscopy, SEM, and TEM. In addition, we converted m-SiO₂ to mesoporous silicon (m-Si) by using magnesiothermic reduction. Si can make an amplified signal by DNP, one of the hyperpolarization phenomena, so that it can be used for MR imaging probe. Consequently, silicon-coated gold nanoparticle (Au NPs@Si) can be used for dual imaging, SERS and MR imaging. Moreover, Au NPs have been used for thermal therapy for cancer as photo-thermal agents for a long time and mesoporous silicon can be used for drug delivery. Therefore, Au NPs@Si can be used for dual therapy, both thermotherapy through the Au NPs and chemotherapy through mesoporous silicon. As a result, we developed Au NPs@Si as the probe for dual therapy and dual imaging for cancer diagnosis and therapy.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-42

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:43, Chair: Wonryeon Cho

Synthesis of Porous Silicon and Carbon Nano-spheres as Hyperpolarized MRI Probes for Cancer Diagnosis

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Silicon and carbon based nano-spheres have been attracting a lot of interest in the field of biomedical applications due to their biocompatibility and biodegradability in vivo, as well as their flexible surface modifications. Here, we synthesized and investigated porous silicon (PSi NPs) and carbon nano-spheres (CNS) as hyperpolarized MR imaging probes. The Si NPs and CNS have many great benefits to the hyperpolarized MR imaging. Since core regions of the crystalline nano-spheres are mostly protected from a main relaxation source, such as paramagnetic centers existing at surface defect sites, these nano-spheres show extremely long depolarization times (usually longer than 30 mins), resulting in high MR image contrast with minimum or no background signals. In addition, paramagnetic centers on the surface defect sites play a pivotal role in generating MR signal enhancements induced by dynamic nuclear polarization (DNP) processes, thereby not necessary to add external radical sources. Two different synthetic approaches were demonstrated in order to produce PSi NPs and CNS. (1) Magnesiothermic reduction of porous silica (synthesized by modified stöber method with CTAB template) was processed in order to yield PSi NPs. (2) CNS was synthesized through the polymerization process of dopamine. Several spectroscopic and microscopic results suggest that the synthesized PSi NPs and CNS can potentially be utilized as biocompatible and targetable contrast agents for hyperpolarized MRI researches.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-43

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:45, Chair: Wonryeon Cho

Determination of Fenpyroximate from Honey by LC-MS/MS

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Fenpyroximate is one of the insecticides used in beekeeping farms. This may remain in honey, which is regulated and banned in some countries. Honey have a complex matrix and therefore, it proceeded by combining Liquid-Liquid Extraction (LLE) and Solid Phase Extraction (SPE) for clean-up and concentration. The parameters for clean-up and concentration of the sample were optimized and validated. The parameters such as pH of sample, type of SPE cartridge, volume of extraction solvent, sample volume, volume of elution solvent, type of elution solvent were evaluated. were optimized. The chromatographic separation by LC-MS/MS system was achieved on an InfinityLab Poroshell 120 EC-C18 (3.0 mm i.d. × 50 mm length, 2.7 μm particle size) column using isocratic elution with water and acetonitrile (30:70). Ionization of the analyte was done by electrospray ionization (ESI) and quantitation was performed by multiple reaction monitoring (MRM). The limit of detection (LOD) and limit of quantitation (LOQ) from the spiked sample were 1.56 and 5.00 μg/kg respectively. The accuracy and precision in the working range (5.00-50.0 μg/kg) were 87.99-119.06 % and 0.68-14.29 % (RSD), respectively. The correlation coefficient (r^2) for the linear equations was obtained in the range of 0.9914-0.9977. The established method was applied to monitor thirty types of commercially available honey.

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Code: ANAL1.O-44

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:47, Chair: Wonryeon Cho

Analytical Platforms Employing LC-MS for Glycosylation Assessment of Therapeutic Glycoprotein

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Glycosylation of a therapeutic protein can significantly affect drug's stability, immunogenicity, PK/PD, and bioactivity. Therefore, glycomic analyses are necessary to assess biotherapeutic quality and biosimilar similarity. Current glycome analyses involve the use of complementary methods for assessing specific glycosylation attributes including glycan composition and structure, abundance, and glycosylation site with microheterogeneity. Here, we demonstrated a stepwise approach using MS platform for glycomic characterization, namely glycan analysis by glycomic approach, site-specific analysis using glycoproteomic approach, and intact protein analysis. Two representative therapeutic glycoproteins, interferon-beta-1a (IFN- β 1a) and trastuzumab, were used to compare the performance (results) of different analytical platforms. Interferon- β -1a (IFN- β 1a) possessing single N-glycosylation site was used for this study. IFN- β 1a and trastuzumab were prepared and analyzed using three independent analytical platforms. First, in intact protein analysis, the standards were desalted using 10K MWCO filters. Without further purification or enrichment IFN- β 1a was directly injected onto the nano LC C8 chip/Q-TOF MS. For glycopeptide approach, the standards were digested with pronase E and enriched and fractionated according to size and polarity by graphitized carbon solid phase extraction (GCC-SPE). In parallel, N-glycans were released from therapeutic proteins by PNGase F and then selectively enriched by GCC-SPE. The enriched glycopeptides and glycans were chromatographically separated and analyzed by nano LC PGC chip/Q-TOF MS, respectively. Regardless of analytical platforms, glycosylation profiling in both qualitative and quantitative analysis showed high correlation ($R=0.91\sim0.99$). Each platform showed different strengths and weaknesses, providing different levels of information on glycosylation. The results would be used as the reference for stepwise glycomic characterization during the development & production stage of biotherapeutics.

120th KCS General Meeting & Exhibition

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL1.O-45**

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:49, Chair: Wonryeon Cho

Indolocarbazole-Based Receptors: Synthesis, Characterization and Anion Sensor Applications

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Recently neutral anion receptor molecules have attracted much attention because anions play an important role in a wide range of chemical, medical, environmental and biological processes. In this study, we report a new series of indolocarbazole-based receptor molecules for effective anion sensing. The new anion receptor molecules were synthesized efficiently through photochemical reactions, and their abilities to recognize different anions were fully investigated by ¹H-NMR, UV/vis absorption and photoluminescence spectroscopy.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL1.O-46

Area: Oral Presentation of Young Analytical Chemists I

Type: Oral Presentation, Time: THU 10:51, Chair: Wonryeon Cho

Classification of glycoproteins by pattern identification in traditional Korean medicine (TKM) in human plasma from lung cancer patients

Jihoon Shin, jinwook lee, Min-gyu youn, miseon jeong, Jeonghoon Kang, Wonryeon Cho *

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Patients have difficulties in seeking treatments based on Traditional Korean Medicine (TKM) because of the lack of standardized diagnosis. This study is a preliminary research for patient-specific TKM aiming at the discovery of biomarker for lung cancer diagnosis using the proteomics approach. Glycoproteins are well-known to be associated with diseases (especially cancers) and can be used as biomarkers for corresponding diseases. Six groups (EX, ES, EN, RX, RS and RN) from Lung cancer patients are independently analyzed through glycoproteomics approach based on the pattern identification in TKM. This lead to (1) establish the standardized methodology with proteomics for the pattern identification of lung cancers under the framework of TKM; (2) discover lung cancer biomarkers using TKM and then develop in vitro diagnostic kits for lung cancers that optimize these biomarkers to establish patient-specific TKM for further treatment.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-1

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:00, Chair: Sang Yun Han

Multimodal analysis of Polymer Blending (ABS/Nylon6) during Reliability Test: Mechanical and chemical analysis

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Blends of nylon 6 with acrylonitrile–butadiene–styrene (ABS) materials were prepared and investigated over a change of composition and mechanical strength during the reliability test under high temperature and humidity condition (50°C/90%RH ~ 4 weeks). The morphological change of the injection molded specimens were also observed before and after reliability test by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The change of mechanical properties were also investigated from micro to nanoscales during the reliability test; tensile strength measurement by universal testing machine and nanometer force measurement by atomic force microscopy. Under the reliability condition after 1 week, tensile strength of the sample were reduced by around 20% and the same trend of nanometer force changes were observed at the mapping image by AFM. The bulk and surface chemistry under the condition were also compared to understand the chemical degradation. Poly dispersity Index (PID) by gel permeation chromatography decreased by around 6% while surface chemistry by FTIR were not much changed. Herein, we present the degradation of the polymer blending during the reliability test using multi scale analytical tools.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-2

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:10, Chair: Sang Yun Han

Changes of Saliva N-glycome after Death: A Proof-of-Concept Study for Determining Time of Death

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The estimation of time since death (TSD) is the crucial part for investigations of the suspicious death in forensic science. However, standard methods of TSD estimation are easily confounded by extenuating circumstances and/or environmental factors. Therefore, a panel of TSD markers obtained from more acceptable and accurate method is necessary to definitely determine the time of death. Saliva, one of the vital fluids encountered at crime scenes, contains various glycoproteins which are highly affected by biochemical environment. Here, we investigated saliva N-glycans between live and dead rats to determine the alteration of N-glycans using animal model system due to the limitation of saliva collection from recently-deceased humans. Rat saliva samples were collected both before and after death. N-glycans were enzymatically released by PNGase F without any glycoprotein extraction. Released native glycans were purified and enriched by PGC-SPE. About 100 N-glycans were identified, profiled, and structurally elucidated by nano LC/MS and tandem MS. Sialylated N-glycans were exclusively present in abundance in live rat saliva while non-sialylated N-glycans including LacdiNAc disaccharides were detected in high level following death. Through in-depth investigations using quantitative comparison and statistical analysis, 14 N-glycans significantly changed after death were identified as the potential marker candidates for TSD estimation. This proof of concept study demonstrated the feasibility of saliva glycosylation for estimating time of death, with obvious forensic applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-3

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:20, Chair: Sang Yun Han

Phytochemical, Pharmacological and Cytotoxic Characteristics of a Bioactive Compound Isolated from the Aerial Part of *Stenochlaena palustris* Bedd

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The ethanolic extract of *Stenochlaena palustris* Bedd. (Blechnaceae) was investigated for phytochemical, pharmacological and cytotoxic properties in a dose-dependent manner. The gummy concentrate obtained from ethanolic extraction was designed as crude extract with a yield of 17.6% for investigation. Phytochemical study revealed the presence of glycosides, flavonoids, saponines and alkaloids. The antioxidant property was evaluated by both qualitative test (using thin layer chromatography) and quantitative test (DPPH scavenging assay, total phenolic content assay, total flavonoid content assay, total tannin content assay, reducing power assay, nitric oxide scavenging assay, hydrogen peroxide scavenging activity, hydroxyl scavenging activity). In the quantitative assay, the extract showed dose-dependent free radical scavenging activity ($IC_{50} \sim 30.5 \mu\text{g/mL}$) which is comparable to that of standard ascorbic acid ($IC_{50} \sim 7.08 \mu\text{g/mL}$). Analgesic activity was investigated on Swiss Albino mice by hot water tail immersion method where extract at dose of 200 mg/kg and 400 mg/kg exhibited significant ($P < 0.05$ and $P < 0.001$, respectively) inhibition of pain by 157.27 and 146.15 after 120 and 180 minutes respectively while the standard drug Diclofenac Na inhibition was found to be 217.67 after 180 minutes at a dose of 25 mg/kg body weight. A linear correlation was found between mortality rates of brine shrimp with increased sample concentration in cytotoxicity test. The results tend to suggest that the plant contains active constituent(s) responsible for the mentioned activities and supports the traditional uses of this plant which also require further investigations to isolate bioactive compounds and to identify its underlying mechanisms.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-4

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:22, Chair: Sang Yun Han

Electrochemical immunoassay for amyloid-beta 1-42 peptide in biological fluids interfacing with a gold nanoparticle modified carbon surface

Hye Jin Lee^{*}, Kyung Min Kim, Suhee Kim

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In this poster, an electrochemical immunosensor involving the formation of a surface sandwich complex on a goldnanoparticle (NP) modified screen printed carbon electrode (SPCE) is demonstrated for the femtomolardetection of amyloid-beta 1-42 peptide(A β) in both serum and plasma. Both bioreceptors forming the assay are highly selective antibodies for A β , namely antiA β and which possess different binding sites for the Apeptide. In order to improve the sensing performance for complex biological fluidic matrix analysis, different mixed monolayers of thiol modified polyethylene glycol (PEG) and mercaptopropionic acid (MPA) were self-assembled onto the Au NP-SPCE followed by tethering antiA(12F4)to MPA using a heterobifunctional cross linker.

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Code: **ANAL2.O-5**

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:24, Chair: Sang Yun Han

Detection of lung cancer biomarkers using sandwich assay based on surface plasmon resonance

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In this poster, a surface sandwich sensing platform with surface plasmon resonance (SPR) technique is demonstrated to detect lung cancer biomarkers. To quantitatively analyse lung cancer biomarker, sandwich assay platform was developed. Detection was performed via lung cancer biomarkers onto a gold chip surface by the covalent linking, and then the subsequent binding material was followed for SPR sensing. We predict that our method can be further applied to the detection of a number of cancer biomarkers in biological samples.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ANAL2.O-6**

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:26, Chair: Sang Yun Han

Analysis of defect mechanism using Micro-IR

young woong Ahn

Research Team of Total analysis, KCC Central Research institute, Korea

The FT-IR method is fast, sensitive and has the advantage of not being difficult to sample. In addition, the equipment is easy to operate and can be applied to various fields such as chemical structure analysis, quantitative analysis and reaction analysis by attaching various attachments. In the case of Micro-IR, a high-resolution microscope can be mounted on the IR to be used for defect analysis such as garbage and Cratering of coating specimens, analysis of impurity substances in fine areas, image mapping, and interlayer composition analysis of multi-layer structures. In this study, various defective specimens were analyzed and the causes of defects were identified and classified by type. Defects caused by foreign matter, contamination transfer, and film loss were detected the most, and it was confirmed that analysis of the interlayer composition was possible by analyzing the specimen of multi-layer structure

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-7

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:28, Chair: Sang Yun Han

Study on corrosion mechanism and temperature profile of painted specimens by salt spray test (SST)

JAEHEE KIM

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The purpose of this study was to identify the corrosion mechanism of painted steel sheets and to examine the change of temperature. In order to carry out the experiment, the painted steel sheet was prepared as a test group, and each specimen was corroded under different temperature conditions and observed with a Scanning Electron Microscope with Energy Dispersive Spectroscopy (SEM/EDS). However, it is difficult to observe the experiment in the general environment, because the corrosion rate is slow. So we set up the experiment to be smooth through two methods. First, scribe was applied to the specimens to the same extent so that the corrosion reaction proceeded faster. Second, the experimental environment was set so that salt water was sprayed at a constant pressure and speed using a SST (Salt Spray Test) analysis machinery. Through this experiment, it is possible to observe corrosion reaction and the change stage, and to understand the relationship between temperature and corrosion degree.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-8

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:30, Chair: Sang Yun Han

On-Chip Direct Diagnostics based on Grating Coupling of Scattered Nanometals in Evanescent Field Layer

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The grating coupling of a scattered novel nanometals was effectively utilized for direct diagnosis of influenza virus without amplification process. Gold nanopad was used as a substrate for analyzing hybridization of single-stranded DNA (ssDNA) with nanometal tag (silver) by total internal reflection scattering (TIRS) microscopy. The grating separated the scattering signals of the nanotag from that of the substrate and displaced the optical path of the scattered signals to avoid errors caused by numerous acquisitions. This sandwich hybridization based biosensor quantified the target until zeptomolar concentration without interference of background by grating associated TIRS. The detection method is a significant advance in the development of an amplification-free biosensor to greatly reduce the time of sample pretreatment for quantitative screening of influenza A (H7N9) virus.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-9

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:32, Chair: Sang Yun Han

Analysis of Famphur in Honey by Solid-Phase Extraction and GC-MS

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Famphur which is a highly hazardous pesticide classified by WHO, may have adverse effects on humans and environments. But there was no guideline for famphur remaining in honey. In this study, a method for the selective determination of famphur in four kinds of honey using solid-phase extraction(SPE) and gas chromatography-mass spectrometry(GC-MS) was established. 5 g of honey was dissolved in 10 mL of water and transferred to a C18 cartridge preconditioned with ethyl acetate and water. After washing with 2 mL of purified water, and then famphur was eluted with 6 mL of ethyl acetate and determined by gas chromatograph with mass spectrometer(GC-MS). Optimization of solid-phase extraction(SPE) parameters was evaluated by the pH of the sample, the type and volume of the elution solvent. Chromatographic separation was achieved on DB-35MS column(30 m × 0.20 mm × 0.33 μm), and oven temperature was raised from 120 °C to 310 °C at a rate of 25 °C/min, and then maintained for 2 minutes. The injection mode was the split mode(10:1), and m/z 218.0 was used as the quantitative ions in SIM mode. From the established extraction and GC-MS conditions, the limit of detection(LOD) and limit of quantitation(LOQ) in the spiked sample were 2 ng/g and 5 ng/g, respectively. Recovery studies were performed at 5 ng/g, 10 ng/g, 20 ng/g of fortification levels, and accuracy and precision in working range were 63.7-118.4 % and 1.0-27.7 RSD %, respectively. The calibration curves for the quantitative analysis were obtained the concentration range of 5~50 ng/g with correlation coefficients(R²) from 0.9883 to 0.9958. The proposed method was applied to the analysis of famphur in domestic honey samples.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-10

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:34, Chair: Sang Yun Han

Near-infrared fluorescent probes for the detection of alkaline phosphatase activity in-vivo imaging

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Alkaline phosphatase (ALP) is a crucial biological enzyme for osteoblast activity during early osteoblast differentiation, but only few biologically compatible methods are available for its detection. Here, we developed highly selective, sensitive and fast responsive new near-infrared (NIR) fluorescence probes, NIR-Phos 1 and NIR-Phos 2, for the fluorescent detection of ALP. The NIR probes also displayed desired properties such as high stability and selectivity, showing a highly rapid “turn-on” fluorescence response rate completed within 1.5 min, on adding 0.1 U/mL ALP. By taking advantage of the superior properties of the NIR probes, we have demonstrated its utility in real-time monitoring of both the concentration- and time-dependent variations of endogenous ALP in living cells and animals, thereby providing a potentially powerful approach for probing ALP activity in biological systems.

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Code: **ANAL2.O-11**

Area: Oral Presentation of Young Analytical Chemists II

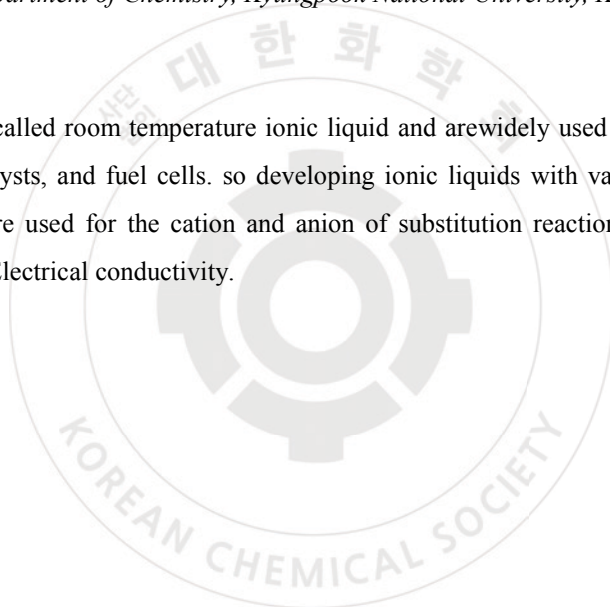
Type: Oral Presentation, Time: FRI 09:36, Chair: Sang Yun Han

Synthesis of Alkaline Ionic Liquids for electrolytes of fuel cells

SONG HA LEE, Hye Jin Lee*

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these ionic liquids are called room temperature ionic liquid and are widely used in various fields besides organic synthesis, catalysts, and fuel cells. so developing ionic liquids with various properties in more easy way. solvents were used for the cation and anion of substitution reaction, and the synthesis was checked by IR, NMR, Electrical conductivity.



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Code: ANAL2.O-12

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:38, Chair: Sang Yun Han

Contemporary Multispectral Three Dimensional Observation of Intracellular Organelles via Enhanced Dark-field Super-resolution Microscopy

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An innovative fluorescence-free super-localization approach for imaging intracellular organelles contacts at three dimension using dual-wavelength enhanced dark field microscopy (EDF). Mitochondria associated endoplasmic reticulum [mito-ER] was imaged by labelling the organelles with plasmon nanoparticles (NPs) of different scattering wavelength. The dual-wavelength synchronized EDF setup allows a concurrent imaging of both organelles under physiological conditions. The three dimensional super-localization of the NPs was achieved by fitting the center coordinates by least-cubic algorithm. The reconstructed super-resolution images resolved controversy over the distance between the intracellular organelles at functional contacts. The distance between the organelles was measured to be 45 nm, the distance fits to be the true feature of the organelles at functional contact site. The results designate to be the novel and reliable approach for the analysis of intracellular organelles at three dimension for accurate information under physiological conditions.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-13

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:40, Chair: Sang Yun Han

High Speed Spiral Scanning Spectrometry for reliable Quantitative Analysis of Ag/GO Nanocomposite SERS substrate

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Surface enhanced Raman spectroscopy (SERS) is a sensitive analytical tool in which weak Raman signal are enhanced by localized surface plasmon of noble metal nanoparticles or nanocomposites. In plural recent studies, analytical capability of SERS method, such as reproducibility and uniformity, has been examined with lithographic patterns, size controlled nanoparticles, and colloidal self-assembly. For quantitative SERS measurement, it is required to overcome the interference from the homogeneity substrates and the dispersity of analyte. In this study, we developed high-speed spiral scanning spectrometry for reliable quantitative analysis using flexible SERS substrate. It is a method of measuring whole analytes dispersed on a substrate by rotating and translating a 2-D cylindrical substrate. We measured crystal violet dye on flexible Ag/GO substrate using spiral scanning method. It showed a quantitative analysis curve, high sensitivity and ultra-uniformity. In addition, flexible SERS substrates can be applied to various analytical fields.

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Code: ANAL2.O-14

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:42, Chair: Sang Yun Han

The electron transfer interaction between mediator and enzyme onto the electrode

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Multi-walled carbon nanotubes (MWCNTs) were modified with polydopamine (PDA) to composite the PDA@MWCNTs onto surface of MWCNTs for hydrophilicity. MWCNTs were homogeneously covered with a biocompatible PDA by a simple dip-coating approach in weak base solution. We prepared the PDA@MWCNTs using ultrasonication and stirring method in Tris-HCl buffer solution (pH 8.5). And the [Ruthenium(4,4'-dimethoxy-2,2'-bipyridine)₂Cl₂] ([Ru(dmo-bpy)₂Cl₂]) was synthesized by refluxing in ethanol to confirm the electron transfer effect with glucose oxidase (GOx). And then, we immobilized the [Ru(dmo-bpy)₂Cl₂] with GOx and poly(ethylene glycol) diglycidyl ether (PEGDGE) onto PDA@MWCNTs modified SPCEs. We investigated the electron transfer behaviors of our electrode using cyclic voltammetry (CV) amperometry. The results suggested that the efficiency of electron transfer between enzyme and mediator is important.

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Code: ANAL2.O-15

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:44, Chair: Sang Yun Han

Simultaneous Detection of Thyroid Hormones based on Multi-Immunoreaction by Dual-Wavelength Capillary Electrophoresis

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A novel dual-wavelength capillary electrophoresis (CE) technique with laser-induced fluorescence (LIF) detection has been investigated for the simultaneous separation and determination of thyroid stimulating hormone (TSH), thyroxine (T4), and triiodothyronine (T3). Thyroid hormones have been reported to influence various diseases such as thyroidectomy, thyroiditis, and hypothyroid. Thus, measurements of T4, T3, and TSH are helpful for the clinical evaluation of thyroid function. In this study, immunoreaction and biotin-streptavidin interaction were developed for highly sensitive detection of thyroid hormones as a function of separation efficiency and migration time. Various factors such as the pH of running buffer, separation voltage, and effective length were also examined in order to determine the optimum CE conditions. All three of standard thyroid hormones were analyzed within 3.2 min in 25 mM Na₂B₄O₇-NaOH buffer (pH 9.3) without losing resolving power under optimal conditions, which were 1,000-100,000 times more sensitive than other previous detection methods. Moreover, the CE with LIF detection method also successfully applied to the analysis of real human blood samples. As a result, the immunoreaction-based CE method with LIF detection is an effective, rapid analysis technique for highly sensitive detection of thyroid hormones related to thyroid gland disease.

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Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:46, Chair: Sang Yun Han

Ultra-sensitive Immunodetection of Cancer Antigen 125 based on Enhanced Plasmonic Scattering of Nano Probe by Dual-mode Wavelength-dependent Enhanced Dark-field Super-resolution Microscopy

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A ultra-sensitive immunodetection was achieved for the biomarker cancer antigen 125 (CA125), which was developed based on selected enhanced detection immunotag by dual-mode wavelength-dependent enhanced dark-field (EDF) microscopy. For simultaneous dual-detection, an color digital camera and electron multiplying cooled charge-coupled device camera were used for quantitative and qualitative analysis, respectively, based on the dark-field scattering images. To increase the efficacy of the scattering signal, various size of different plasmon nanoparticle (i.e., gold nanoparticles, 5 nm, 12 nm, 20 nm, 100 nm and 250 nm; silver nanoparticles, 20 nm, 30 nm, 40 nm, 80 nm and 100 nm) were used as the detection tags and investigated with wavelength dependence of the light source, and the quantum efficiency of the electron-multiplying charge-coupled device camera, 40-nm silver nanoparticle (SNP) was selected as an optimum fluorescence-free probe. CA125 was screened at single-molecule level and quantitatively analyzed by measuring the scattering signals of 40-nm SNP on gold-nanodots arraychip. CA125 was screened at single-molecule level and quantitatively analyzed with lowest possible possible LOD ($4 \text{ } \mu\text{g/mL}$, S/N = 3) and a wide dynamic detection range of $4 \text{ } \mu\text{g/mL}$ -80 U/mL ($R = 0.9935$), which was a over the 100 times lower LOD and wider dynamic range than previous researches. Dual-mode EDF based optical property of the plasmon scattering signal of metal nanoparticles allowed us for a of disease related biomolecules at single-molecule level for early diagnosis of life threatening diseases.

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Code: ANAL2.O-17

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:48, Chair: Sang Yun Han

Size-based fractionation and characterization of starch granules using split flow thin cell (SPLITT) and gravitational field-flow fractionation (GrFFF)

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Starch is obtained from cereals (corn, potato and rice), and is used in food, paper, mining industries, and in the production of adhesives. Starch granules from various botanical sources vary widely in the granular size and shape as well as in the composition of amylose, amylopectin and protein, thus leading to differences in functional properties and industrial applicability. In addition, size of starch granules has an important influence on the enzymatic reaction. The sieving may be used for size-based fractionation of granules. However it may induce damage of starch granules by mechanical force. The split flow thin cell (SPLITT) is a separation technique that provides fractionation of a polydispersed sample into two size fractions. SPLITT uses an open channel, and thus mechanical damages could be minimized. It can also be used in a large scale as the sample can be fed continuously. In this study, SPLITT was employed for a size-based fractionation of various starch granules (corn, potato) in a large scale. The SPLITT fractionation results were checked by optical microscope (OM) and gravitational field-flow fractionation (GrFFF). Then the size-fractions of the starch granules were analyzed by differential scanning calorimetry (DSC). Results from DSC suggested that the composition of the starch granules may vary with their sizes and types.

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Code: ANAL2.O-18

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:50, Chair: Sang Yun Han

Variation of separation efficiency of glycogen and pullulan with channel type in field-flow fractionation (FFF)

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Field-flow fractionation (FFF) is a family of tools for the separation and characterization of particles and polymers. It has a broad dynamic range, and the utilization of an open channel requires no packing material, minimizing problems of sample adsorption, degradation and loss than in size exclusion chromatography (SEC). Frit inlet asymmetrical flow field-flow fractionation (FI-AsFIFFF) is a modified form of the asymmetrical field-flow fractionation (AsFIFFF) technique. Relatively higher carrier flow through the frit relative to the sample injection flow compresses the incoming sample band toward the accumulation wall of the channel. The main advantage of FI-AsFIFFF is to bypass the focusing step for relaxation in FIFFF that are normally carried out by stopping the carrier flow for a period of time to establish an equilibrium condition of the sample components. In this study, the separation efficiencies such as resolution, plate height and recovery were compared between AsFIFFF and FI-AsFIFFF channel using glycogen and pullulan. It was found that FI-AsFIFFF yields higher sample recovery than AsFIFFF. However, the resolution of FI-AsFIFFF was lower than that of AsFIFFF (about half). The resolution was increased with increasing the cross flow rate in both channels. Results also indicated that the resolution, plate height and the sample recovery changes with the type of samples. It seems a care needs to be taken in choosing the channel type in FFF studies.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-19

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:52, Chair: Sang Yun Han

Effect of light on size of *chlorella sorokiniana* and production of glutathione using gravitational field-flow fractionation (GrFFF)

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chlorella sorokiniana (or simply, *chlorella*) is one of single-cell green microalgae and has the size range of 2~10 μm . It plays an important role in food as it provides a rich source of carbohydrates, vitamins and proteins. It can also produce the glutathione, which is one of important antioxidant in plants, animals, fungi and some bacteria. The antioxidant-production capacity of the *chlorella sorokiniana* is determined by various parameters including pH, temperature, and the presence of light. Previous studies have been mainly focused on the application of the *chlorella*, and basic studies on the relationship between the antioxidant-production capacity of the *chlorella sorokiniana* and these parameters are insufficient. In this work, the change in the size of the *chlorella sorokiniana* with the presence of light was studied, and then the effects of the size, the presence of light, and incubation time on the capacity of the *chlorella sorokiniana* for production of glutathione were investigated. The size of *chlorella sorokiniana* was determined using an optical microscopy (OM) and gravitational field-flow fractionation (GrFFF). GrFFF is a gentle elution-based separation technique that is known to be useful for separation of micron-sized particles. The glutathione produced from *chlorella* was analyzed quantitatively using a UV/Vis spectrophotometry. Both the size and number of *chlorella sorokiniana* were increased with increasing incubation time until 96 hours, and then were remained constant. The concentration of glutathione also was increased with the incubation time until 96 hours, after which was decreased.

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Code: ANAL2.O-20

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:54, Chair: Sang Yun Han

Identification of behavior of synthesized Sm_2O_3 particles in goldfish

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Rare-earth nanoparticles are generally harmless in the environment, and could be utilized as a tracer for circulation process of nature. The rare-earth nanoparticles can be identified (or analyzed) by gamma ray irradiation, as they are decomposed by the gamma ray irradiation to yield radioactive rare-earth isotopes, producing their own characteristic signals. Gamma-ray irradiation is known to be highly sensitive for analysis of samples of trace concentrations. In this study, samarium oxide (Sm_2O_3) nanoparticles were synthesized by a sono-chemical method, and were analyzed using various techniques including asymmetrical flow field-flow fractionation (AsFIFFF), dynamic light scattering (DLS), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD) and inductively coupled plasma-mass spectroscopy (ICP-MS). AsFIFFF and DLS were used to determine the size distributions of the Sm_2O_3 particles. EDX and XRD were used to determine the chemical composition of nanoparticles. The presence of samarium was confirmed by the XRD and EDX results. The AsFIFFF and DLS results showed the Sm_2O_3 nanoparticles have sizes ranging about 20 ~ 30 nm. The Sm_2O_3 nanoparticles were fed to gold fish, then the concentration of the particles in various organs of the gold fish were analyzed using ICP-MS.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-21

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:56, Chair: Sang Yun Han

Optimization of liquid chromatography mass spectrometry (LC/MS) for the analysis of the ganglioside isomers

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Gangliosides are acidic glycosphingolipids which contain sugar chains with a variety of sialic acid residues. There are hundreds of variations in ganglioside structures based on compositions and structures of oligosaccharide head groups as well as compositions of ceramide cores. However, most LC/MS studies did not include separation of these structural isomers. Therefore, we tried to optimize LC conditions for resolving ganglioside isomers and we specifically focused on developing separation conditions for resolving structural isomers of disialogangliosides, designated to GD1a and GD1b, which are known to be major species in mammal brains. Through optimization processes, we developed an effective LC condition with a conventional C18 column and an appropriate salt additive. And we applied the optimized LC/MS method to the analysis of the total ganglioside extract from porcine brain and successfully analyzed individual isomers of di- and tri- gangliosides.

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Code: ANAL2.O-22

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 09:58, Chair: Sang Yun Han

Investigation of sample preparation and analysis methods for profiling organic chemicals and metals in teeth

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Recently, due to its specific structure and growth pattern, deciduous teeth have been proposed to be retrospective temporal biomarkers for exposomics researches which try to assess comprehensively environmental exposures from the fetal period onwards. However, sample preparation and analysis steps for teeth samples have not been explored extensively and need to be standardized. In this study, we investigated various sample preparation procedures and mass spectrometric methods for profiling organics and metals present in teeth samples. In order to evaluate sample preparation procedures including sampling, pulverization, incubation, and extraction, we employed paper spray ionization (PSI) mass spectrometry (MS), paper cone spray ionization (PCSI) MS, and MALDI MS. In addition, we tested various LC/MS methods for organic chemical analysis and laser ablation-based elemental mapping methods for spatially resolved metal analysis.

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Code: ANAL2.O-23

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:05, Chair: Sang Yun Han

The structural characterization of disease related human transmembrane proteins using the NMR spectroscopy

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Human transmembrane proteins (hTMPs) play essential roles in cellular metabolism, participating in processes such as ion transport, nutrient uptake, signal transduction, and intercellular communication. However, aggregation or misfolding of hTMPs due to unwanted mutations of amino acid sequences or errors in the folding process leads to an increase in various human diseases. Therefore, we aim to create new treatments that can inhibit or eliminate these changes. In this research, we tried to identify the structure of human amyloid- β (hA β) and human melanocortin-4 receptor (hMC4R). The hA β transmembrane protein shows that the non-fibrillar hA β s form the Ca²⁺-permeable ion channel in the cell membrane and these channels can disrupt the normal cellular calcium homeostasis. It plays an important role in pathogenesis of dementia and Alzheimer disease. The human melanocortin-4 receptor (hMC4R) has been highlighted because it is central regulator of body weight. Heterozygous mutations related in genetic cause of severe obesity. We succeed to produce the transmembrane domain of the hA β and second transmembrane domain of the wild-type hMC4R and mutant hMC4R. In cases of the wt/m-TM2 purification, we used sodium dodecyl sulfate (SDS) because of their hydrophobicity. Since SDS binds so strongly to protein, it interferes with biophysical techniques used for characterization of wt/m TM2. Thus, we developed the removal methods of SDS to obtain high quality of purification for wt/m-TM2. Highly purified proteins were applied to several analysis techniques like PAGE, CD, MASS, solution and solid-state NMR spectroscopy. In addition, we could get ¹H-¹⁵N 1D, 2D SAMMY and SAMPI spectra using home-built solid-state NMR probe.

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Code: ANAL2.O-24

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:07, Chair: Sang Yun Han

Diverse home-built solid-state NMR probes for specific purposes

jiho jung, Ji Sun Kim , YONGAE KIM*

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The solid-state NMR has been used to investigate insoluble materials in advanced industrial site. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. We will 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 narrow-bore(NB) ^1H - ^{15}N solid-state NMR probe for these electrically lossy samples. Li-ion battery and LCD panel have been grown up rapidly as a front-runner in technology-intensive industry. Their microstructural changes are the reason of battery efficiency drop and defective pixel. We will also present a home-built 500 MHz NB ^{19}F - ^{13}C solid-state NMR probe with flat-square coil for analyzing LCD panel and 600 MHz NB ^{19}F - ^7Li solid-state NMR probe 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. These two probes provide high efficiency and good RF homogeneity. And finally we will introduce our recent commission task project "Development of sample dependent Solid-state NMR probe for the analysis of nanomaterials". The ^{19}F - ^{13}C solid-state 400 MHz NB probe was made and quality test was in progress.

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Code: ANAL2.O-25

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:09, Chair: Sang Yun Han

Development for simultaneous purification of nerve agent metabolites using MB-Ab complex and affinity gel and application to nerve agent inhibited rhesus monkey plasma

JinYoung Lee^{*}, JIHYUN KWON, Yong Han Lee

Agency for Defense Development, Korea

A sensitive method for the purification and determination of two protein adducts, organophosphorus (OP)-BuChE and OP-albumin adducts, in a single sample using a simultaneous sample preparation method was developed and validated using liquid chromatography-tandem mass spectrometry (LC-MS/MS). First, we isolated O-ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (VX) and O-pinacolyl methylphosphonofluoridate (soman, GD)-BuChE adducts using an immunomagnetic separation (IMS) method and the HiTrap Blue affinity column was subsequently used to isolate and purify VX and GD-albumin adducts from the plasma of rhesus monkeys exposed to nerve agents. Additionally, we examined the time-concentration profiles of two biomarkers, VX and GD-nonapeptide and VX and GD-tyrosines, derived from OP-BuChE and OP-albumin adducts up to 8 weeks after exposure. Based on the results, we determined that VX and GD-tyrosine is more suitable than VX and GD-nonapeptide as a biomarker owing to its longevity. This integrated approach is expected to be applicable for the quantification of other OP-BuChE and OP-albumin adducts in human plasma, thus serving as a potential generic assay for exposure to nerve agents. Keywords: immunomagnetic separation; chemical warfare agent; butyrylcholinesterase; albumin; UPLC-MS/MS

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Code: ANAL2.O-26

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:11, Chair: Sang Yun Han

Optimization of Preparation Condition for Analysis of Statins and Fibrates Adulterated in Oil type Dietary Supplements

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The incidence of hyperlipidemia, which is one of cardiovascular diseases, has increased due to changes in westernized dietary habits of modern humans. Fibrate derivatives and statins which are HMG-CoA reductase inhibitors are representative drug components for treating hyperlipemia. However, these medicines may cause various side effects due to long-term dose. For this reason, consumers purchase dietary supplements such as form of oil soft capsules containing natural omega-3 fatty acids. Sometimes, there are cases in which unauthorized components is added to improve their pharmacological efficacies. Thus, it is necessary to investigate the illegally adulterated components in dietary supplements using the optimized preparation and analytical methods. In this study, to find out the optimum preparation condition for oil soft capsules, normal hexane (A) and 70% MeOH (B) mixture were selected as liquid-liquid extraction (LLE) solvents. The ratios of A and B were changed as follows; 3:1, 2:1, 1:1, 1:2, and 1:3 (v/v), respectively. After preparation, all samples were analysed by ultra performance liquid chromatography (UPLC), in triplicate. In conclusion, only the recovery of 1:1 ratio was confirmed at 80 ~ 120%. Therefore, a suitable ratio of the LLE solution for detecting the statins and fibrates adulterated in oil type dietary supplements is 1:1, and it is considered that can be used as a more effective preparation condition.

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Code: ANAL2.O-27

Area: Oral Presentation of Young Analytical Chemists II

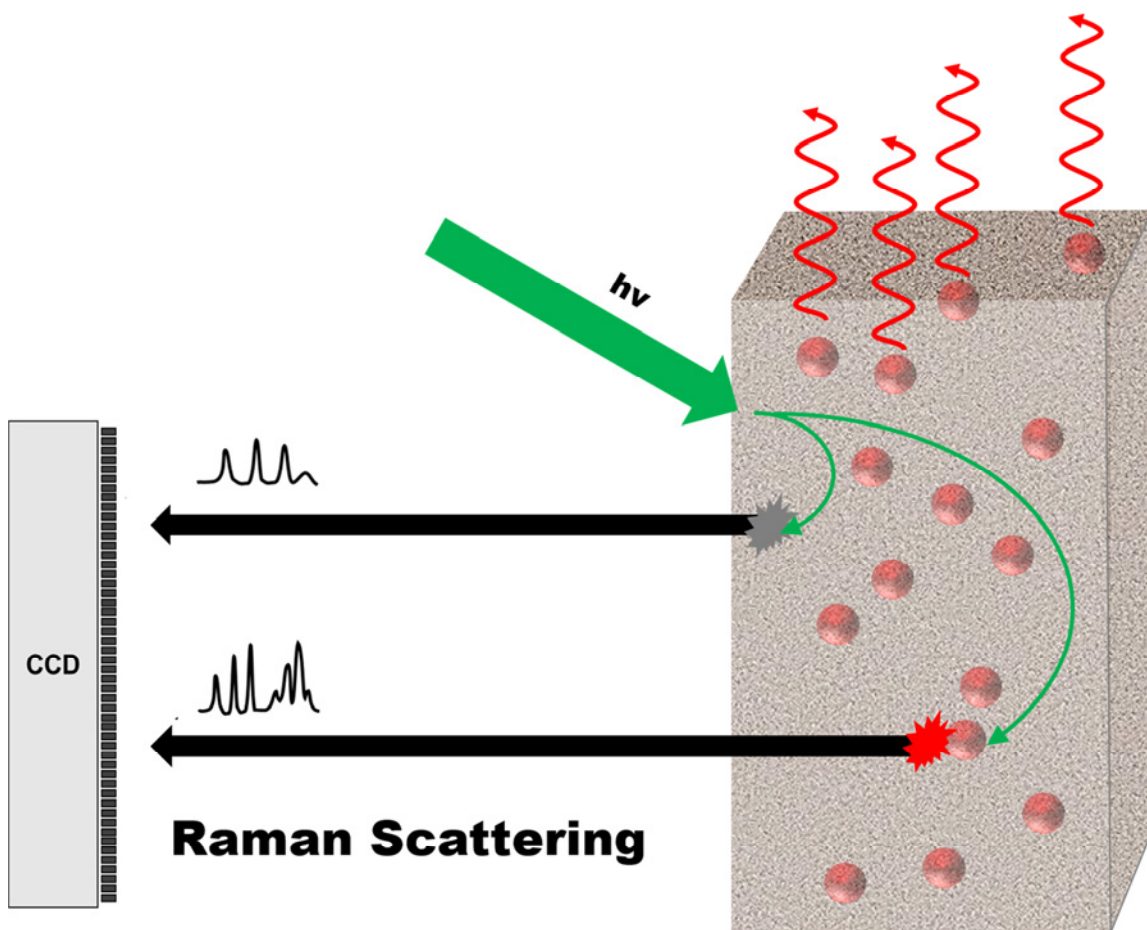
Type: Oral Presentation, Time: FRI 10:13, Chair: Sang Yun Han

Wide-depth Spatially offset Raman Spectroscopy for Detecting Hazardous Chemicals in Building Materials

Youngho Cho, Chan Ryang Park, Hyung Min Kim^{*}

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Toxic chemicals inside building materials must be detected early to prevent secondary damage because the chemical have long-term harmful effect on the human body. Although deep Raman spectroscopy is a potential candidate for inside harmful materials detection, it is very difficult to distinguish the Raman signal of the inside chemicals from the background signal of surrounding building materials. In this study, we developed wide-depth spatially offset Raman spectroscopy (W-SORS) coupled with a processing algorithm to identify inside chemicals. Furthermore, we proposed a method of measuring the thickness of an external building materials through signal processing of the W-SORS spectral slope.



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Code: ANAL2.O-28

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:15, Chair: Sang Yun Han

Fast Direct Apolipoprotein E Genotyping for Alzheimer's by Multi-channel Microchip Electrophoresis

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A direct apolipoprotein E (apoE) genotyping-based multi-channel microchip electrophoresis (ME) method was developed for fast high-throughput screening of Alzheimer. The target apoE polymorphism genes (i.e., 112 bp, 253 bp, 308 bp, 444 bp, and 514 bp DNA) were amplified by only 10 cycles of one-step multiplex polymerase chain reaction (PCR) from whole blood without DNA extraction. The amplified target DNA fragments were detected in 20 s by a programmed electric field strength (PEFS)-based single-channel ME. According to the optimum conditions of single-channel ME, target DNA fragments were separated using various multi-channel ME with three and five parallel channels, which simultaneously detected within 20 s without any loss of resolving power or reproducibility. The proposed multi-channel ME-PEFS assay technique provides a simple and accurate method for fast high-throughput screening of Alzheimer's disease, which can be simply apply to more large number of parallel channels for more high-throughput screening.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-29

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:17, Chair: Sang Yun Han

Identification of Diverse Types of Monosaccharide Derivative Isomers By Host-guest Complexation with Cucurbit[7]uril

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Distinguishing constituent monosaccharides in target carbohydrate using mass spectrometry (MS) remains challenging due to their undistinguishable fragmentation patterns induced by their isomeric structures and similar physical properties. Although a carbohydrate is composed of diverse monosaccharide/monosaccharide derivative species, previous methods focused on one or two types of monosaccharides and monosaccharide derivatives. Therefore, it is necessary to invent a novel approach to be developed as a comprehensive method for identification of diverse types of monosaccharides and monosaccharide derivatives. Our study reveals that the combination between host-guest and gas-phase chemistry is effective for identifying diverse types of monosaccharide derivative isomers. Four different types of monosaccharide derivative isomers were investigated herein as target monosaccharide derivative species. A host molecule, cucurbit[7]uril (CB[7]), was utilized herein due to its high recognition ability in monosaccharides. It was observed that each monosaccharide derivative forms gas-phase complex with CB[7] while most of bindings between the CB[7] and target guests are negligible in aqueous solution. Tandem MS study shows that the monosaccharide derivatives have different fragmentation patterns in their complexes with CB[7], allowing their identification. Structural studies using ion mobility MS and computational calculations suggest that the slight structural differences between the isomers are augmented by their distinct host-guest interactions with CB[7] in the gas-phase. Overall, the present study reveals that our gas-phase host-guest system can be developed as a comprehensive method for qualitative analysis of constituent monosaccharides in target carbohydrates.

120th KCS General Meeting & Exhibition

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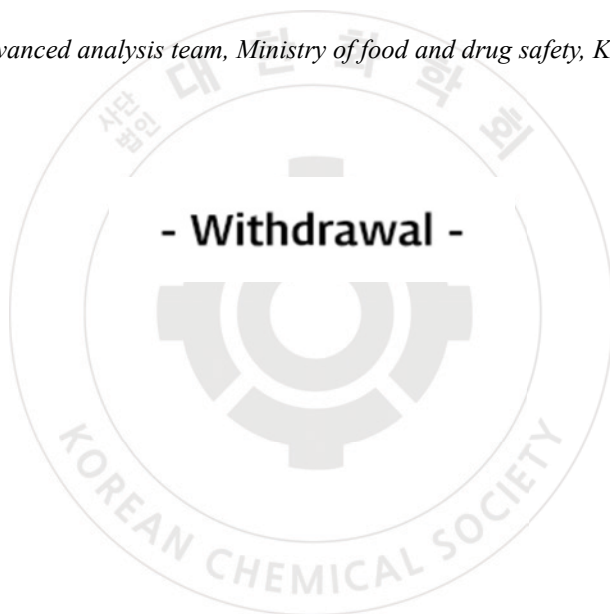
Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:19, Chair: Sang Yun Han

[Withdrawal] Simultaneous determination of 21 tar colors in lipsticks by ultra-performance liquid chromatography

Jun hyoung Kim, GiHaeng Kang, Seongsoo Park, Hoil Kang*

Advanced analysis team, Ministry of food and drug safety, Korea



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-31

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:21, Chair: Sang Yun Han

Potential biomarkers of diabetic kidney disease detected by NMR-based metabolite profiling

Jin Seong Hyeon, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Previous studies described metabolite profiles of diabetic animals; however, they were highly variable because of heterogeneity of the studies. We aimed to characterize the metabolite changes in the early and late stages of diabetic kidney disease to suggest potential biomarkers for early detection and its progression. Metabolite profiling using high-resolution nuclear magnetic resonance spectroscopy and multivariate statistical analysis was performed in *db/db* mice. We compared concentrations of serum and urinary metabolites between *db/m* and *db/db* mice at 8 or 20 weeks of age and investigated whether changes between 8 and 20 weeks in each group were significant. Correlation analysis was used to determine associations between urinary metabolites and urinary albumin excretion. Partial least squares-discriminant analysis score plots showed a significant distinction between *db/m* and *db/db* mice. The metabolic profiles demonstrated significantly increased urine levels of glucose and tricarboxylic acid cycle intermediates, such as fumarate, citrate, and 2-oxoglutarate, at both 8 and 20 weeks in *db/db* mice. These intermediates also exhibited strong positive associations with urinary albumin excretion, suggesting that they may be potential biomarkers for early diagnosis. On the contrary, branched chain amino acid and homocysteine-methionine metabolism were activated early in the disease, whereas ketone and fatty acid metabolism were significantly changed in the late phase of the disease. We demonstrated phase-specific alterations in metabolites during progression of diabetic kidney disease. This study provides insights into perturbed mechanisms during evolution of the disease and identifies potential novel biomarkers for diabetic kidney disease.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-32

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:23, Chair: Sang Yun Han

Highly sensitive detection of lethal infectious pathogen using SERS-based lateral flow assay

Rui Wang, Kihyun Kim, JAEBUM CHOO*

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Effective identification of pathogenic bacteria is important for biodefense. In recent years, microbiological culture and colony counting, polymerase chain reaction (PCR) or immunoassay has been considered as a gold standard for the detection of pathogens including toxin, bacteria and virus. However, these methods cannot meet the requirement of rapid and highly sensitive detection because they need long sample preparation time and have limited detection sensitivity. Therefore, it is still urgent to develop a new method for the rapid and sensitive detection of pathogens for preparedness of bioterrorism. In this presentation, we introduce a new pathogen assay technique using a surface-enhanced Raman scattering (SERS)-based lateral flow assay. Two different antigens, including botulinum toxin A and *Yersinia pestis* have been selected as detection targets. According to our assay results, the limit of detection of botulinum toxin A and *Yersinia pestis* using the SERS-based lateral flow platform was 10 pg/mL and 102 CFU/mL, respectively, which are three orders of magnitude more sensitive than that of commercial rapid kit. Thus, the proposed SERS-based lateral flow assay has a strong potential to be a valuable tool in the early detection of a specific pathogen due to its excellent analytical sensitivity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-33

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:25, Chair: Sang Yun Han

Rapid and sensitive detection of highly risk pathogens using SERS-based lateral flow assay

Kihyun Kim, Rui Wang, JAEBUM CHOO*

Department of Bionano Technology, Hanyang University, Korea

Bioterrorism has been received great concerns after the 2001 anthrax attacks in United States. Highly risk pathogens used in the bioterror are greatly contagious and also have a high fatality. To minimize life damages from bioterror, rapid and sensitive detection methods of specific pathogen is urgently required. To date, various detection methods including direct counting of bacteria, polymerase chain reaction (PCR), and immunoassay have been developed but they do not satisfy the requirements in the field due to complicated sample pre-treatment procedures, long detection time and low sensitivity. To resolve those problems, we recently developed a SERS-based detection technique for the detection of various pathogens. In this poster, we introduce a new pathogen assay method using a SERS-based lateral flow assay. Two different pathogens, *Bacillus anthracis* and *Francisella tularensis* have been selected as detection targets. In the case of *Francisella tularensis*, the limit of detection measured by the SERS-based lateral flow platform was estimated to be 10^2 CFU/mL, which is three orders of magnitude more sensitive than that of commercial ELISA kit. Therefore, the proposed SERS-based lateral flow assay technique has a strong potential to be used as a valuable tool in the early detection of a specific pathogen due to its simplicity and excellent analytical sensitivity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-34

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:27, Chair: Sang Yun Han

Application of gradient generating microdroplet-based chips for rapid and sensitive bioanalysis

Jinhyeok Jeon, JAEBUM CHOO*

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Microfluidic technology have recently emerged as an efficient tool for the study of various chemical or biological reactions. Recently, we reported that high-throughput chemical or biological reactions could be performed in a continuous flow microfluidic channel with an automatic manner. However, there is a “memory effect” problem in the continuous flow system. Samples in the continuous stream could be stacked in the wall of a microfluidic channel, and they may occur unwanted flow hindrance. To resolve this problem, we recently developed a novel gradient microdroplet system. In this system, the sample stacking problem can be solved since two-phase liquid/liquid segmented flow reduces the memory effect. A serial dilution of reagent can be achieved in a stepwise manner using microfluidic concentration gradient generators. Then, desired concentrations of a reagent were 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 effects for various concentrations of a reagent.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-35

Area: Oral Presentation of Young Analytical Chemists II

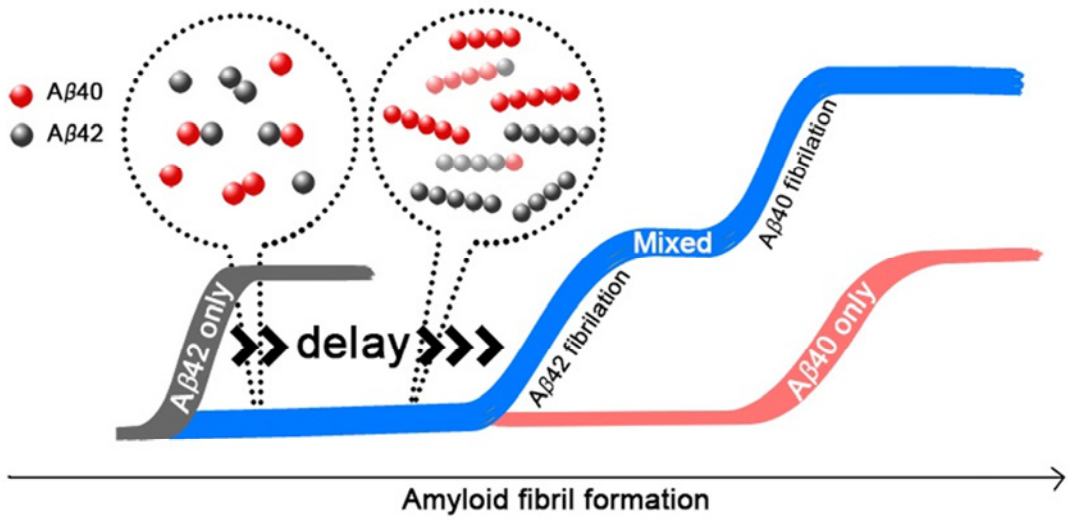
Type: Oral Presentation, Time: FRI 10:29, Chair: Sang Yun Han

Investigation of the homo- and hetero-oligomerization of amyloid- β 1-40 and 1-42 using electrospray ionization mass spectrometry

Chae Eun Heo, Taesu Choi^{*}, Hugh Inkon Kim^{*}

Department of Chemistry, Korea University, Korea

Self-assembly of amyloid- β peptides ($A\beta$) has accepted as an important issue, because the final product of the self-assembly (i.e. amyloid fibrils) is highly relevant to the Alzheimer's disease (AD). Among various $A\beta$ alloforms, $A\beta$ 1-42 ($A\beta_{42}$) and $A\beta$ 1-40 ($A\beta_{40}$) are mainly involved in $A\beta$ fibril formation. The self-assembly mechanisms of $A\beta_{42}$ and $A\beta_{40}$ are known to be different and $A\beta_{42}$ and $A\beta_{40}$ can form hetero-assemblies through their cross-interaction. However, the role of hetero-assemblies of a mixture of $A\beta_{42}$ and $A\beta_{40}$ is not yet fully understood. Thus, characterizing the cross-interaction between $A\beta_{42}$ and $A\beta_{40}$ is crucial for understanding the role of hetero-assemblies during the fibrillation of mixed $A\beta$ peptides. In this research, we demonstrated the influence of the cross-interaction of $A\beta_{42}$ and $A\beta_{40}$ in the early stage of fibrillation. We monitored the fibrillation process of $A\beta_{42}$, $A\beta_{40}$ and their 1:1 mixtures using thioflavin T (ThT) assay and electrospray ionization mass spectrometry (ESI-MS). Then, we further investigated the preference for homo- and hetero- oligomerization of $A\beta_{40}$ and $A\beta_{42}$ using ion mobility spectrometry (IMS) along with solution small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations. Our results suggest that the competitive self-assembly of $A\beta_{42}$ and $A\beta_{40}$ plays a pivotal role in disturbing homo-oligomerization of $A\beta_{42}$ in the early stage of fibrillation.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-36

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:31, Chair: Sang Yun Han

Developed to Overhauser Dynamic Nuclear Polarization Nuclear Magnetic Resonance Systems for Signal Enhancement

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

Nuclear magnetic resonance (NMR) spectroscopy has advantages such as non-destructive observation of molecular structure and dynamics, analysis of amorphous samples, and high selectivity of nuclear species to be observed. However, NMR has the disadvantage of low sensitivity because it uses low energy. In order to overcome the disadvantage of NMR, overhauser dynamic nuclear polarization (ODNP) NMR system which amplifies NMR signals from several tens to several hundred times using the interaction of electron spins and nuclear spins within about 1 nm from the electron spin centers. Therefore, a local region can be designated by selectively positioning the spin markers in the sample. ODNP NMR can be used to measure the diffusion rate of water in a variety of materials and to measure the dependence of binding between protein and water on solvents. In our laboratory, an Electron Paramagnetic Resonance (EPR) spectrometer and NMR components (radio frequency pulse modules, NMR tuning boxes, ODNP NMR probes, etc.) has been assembled together and instrumental optimization for the best amplification is currently in progress.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-37

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:33, Chair: Sang Yun Han

A Method for Quantitative Analysis of Cellular Uptake in Combination Therapy Treating Neuroblastoma

Hong Areum, Min Gyeongseo, Hugh Inkon Kim^{*}

Department of Chemistry, Korea University, Korea

Neuroblastoma is fourth most abundant malignant tumor in childhood which begins when immature nerve cells grow out of control. As Neuroblastoma belongs to heterogeneous disease, chemotherapy has been underway as combination of various anticancer drugs. Therefore, to optimize combination chemotherapy for diverse case, understanding how combination therapy works better than single drug is crucial. However, relevant researches so far have been focused on only combination efficiency in clinical investigation. In this research, we aim to study cellular uptake of combination therapy in correlation to drug efficiency for cancer cells, compared to single drug regimen. Firstly, cell viability test for neuroblastoma cell lines, SK-N-SH and SH-SY5Y, was conducted using each drug in combination therapy to search proper drug treating condition. Also, we tried to develop quantitation method based on mass spectrometry for drug in cell culture media. As a result, we optimized solvent condition for maximizing drug ionization efficiency in mass spectrometry and pretreatment method of culture media to quantify small molecules such as drugs. With aforementioned results, we are currently working on the correlation between treatment efficiency and time-based cellular uptake after using combination or single drug.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-38

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:35, Chair: Sang Yun Han

Metabolic profiling in heart tissue of mice fed atherogenic diet

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¹*Korea Basic Science Institute, Korea*

Atherosclerosis is a leading cause of cardiovascular disease characterized by thickening of the arterial wall resulting from abnormal lipid accumulation. In atherosclerosis model, most of the studies illustrated the mechanism of atherosclerosis in biofluids and/or liver but not in heart. In the present study, we performed metabolic profile in heart tissue during the progression of diet-induced atherosclerosis mouse model using liquid chromatography/mass spectrometry (LC/MS). A lipidomics approach was used to investigate the changes in lipid species in heart tissue from AD mice. Principal component analysis (PCA) plots showed a clear differentiation between normal diet (ND) and atherogenic diet (AD) groups in both positive and negative ion modes. In the PCA score plots, significant discriminations between ND and AD groups was observed in each time point (8 weeks, 16 weeks, and 25 weeks). Cers were significantly decreased in AD group, whereas GlcCers were increased in AD group. Saturated fatty acids including FFA 16:0 (palmitic acid) and FFA 18:0 (stearic acid) were significantly increased in AD, whereas unsaturated fatty acids were decreased. TG species were changed depending on the length of acyl chain and degree of unsaturation. Also we assessed quantitative analysis of suffer-containing amino acid (SAA) metabolites which is related with stearyl-CoA desaturase-1 (SCD1) because SCD1 produces monounsaturated fatty acids from saturated fatty acids. The levels of SAA metabolites in heart tissue were significantly changed in AD mice. This study demonstrates that LC/ MS based metabolic profiling can be used to understand metabolism in heart tissue of diet-induced atherosclerosis animal model and may provide the insight for molecular aspects of cardiovascular diseases.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-39

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:37, Chair: Sang Yun Han

Facile Fabrication of Nanostructured Surfaces Amenable to Laser Desorption/Ionization of Drug Molecules

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

Herein, we present a facile strategy to bring the LDI (laser desorption/ionization) capability onto nanostructured surfaces, which can further be tailored with various surface coatings suitable to individual applications. While the MALDI (matrix-assisted laser desorption/ionization) method has been a powerful tool to ionize thermally labile molecules such as biological and synthetic polymers, the intrinsic use of excess matrixes causes certain limitations on its applications. To overcome the related issues, matrix-free LDI methods have been demonstrated in recent years; in particular, a variety of nanostructures were exhibited for their LDI capability, most of which are unfortunately too special to be prepared by other laboratories. In this presentation, we present a simple and facile strategy of how to get certain surface nanostructures to achieve the LDI capability by using known techniques of surface chemistry. The strategy is based on the thermal mechanism that would promote intact desorption of thermally labile molecules by laser-induced surface heating. The produced LDI nanostructured surfaces can further be decorated by surface coatings to possess the suitable surface properties for individual applications, such as hydrophobic, hydrophilic, and non-fouling properties. All these can be done by simple and known chemistry. In addition, this strategy is applicable to virtually any nanostructured surfaces. In this work, the strategy is demonstrated on conical AAO (anodized aluminum oxide) templates with respect to LDI of drug molecules with moderate molecular weights of 500 to 1000 Da.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-40

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:39, Chair: Sang Yun Han

Metabolomic analysis of polychlorinated biphenyls(PCBs) and organochlorine pesticides(OCPs) exposure in human plasma

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¹*Korea Basic Science Institute, Korea*

Polychlorinated biphenyls(PCBs) and organochlorine pesticides(OCPs) are types of persistent organic pollutants (POPs) known as lipophilic environmental toxins. Accumulation of POPs has adverse effects on both environment and human. However, few studies have assessed their internal exposure to POPs. The objective of this study was to observe the effect by accumulation of POPs in humans and to investigate the associations between POPs levels and metabolic profiles in plasma samples. In this study, concentrations of total 33 POPs including 16 PCBs and 17 OCPs were analyzed from plasma samples of 300 Koreans without occupational exposure to POPs. The sum of the signed ranks of five PCBs and six OCPs, respectively, were used in multivariate regression tools adjusted for age, sex, BMI, education, smoking and alcohol intake. Then, we performed plasma metabolic profiling using ¹H-NMR spectroscopy. We found that PCBs were significantly associated correlated with creatine, glucose, mannose, citrate, and phenylalanine. On the other hands, OCPs were correlated with creatine, mannose, lactate, and phenylalanine. This study suggests that the NMR-based metabolomic approach may provide a promising technique to understand the alteration of human metabolism and to identify potential biomarkers for estimating exposure effect of environmental toxins like POPs.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-41

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:41, Chair: Sang Yun Han

Structure Elucidation and Potential Function study of Microcystin-LR

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The microcystin is a cyclic heptapeptide from metabolites of cyanobacteria in the genera *microcystis*, *anabaeba* as a result of eutrophication. It has been known that microcystin-LR is a potent inhibitor of the catalytic subunits of protein phosphatase-1(PP-1) as well as powerful tumor promoter. The active site of microcystin actually has two metal ions Fe^{2+}/Zn^{2+} close to the nucleophilic portion of PP-1-microcystin complex.

We report the isolation and purification of this microcystin-LR from cyanobacteria (blue-green algae) obtained from Daechung Dam in Chung-cheong Do, Korea. Microcystin-LR was extracted from solid-phase extraction (SPE) sample preparation using a CN cartridge. The cyan bacteria extract was purified to obtain microcystin-LR by HPLC method and identified by LC/MS. The solution structure of this compound was investigated with ¹H-NMR and 2D NOESY experiments were accomplished in DMSO-d₆ and signal assignment of microcystin-LR. On the basis of these distance data, distance geometry and molecular dynamic were carried out to determine the tertiary structure of microcystin-LR.

The detail structural studies that can elucidate the possible role of monovalent and divalent metal ions in PP-1-microcystin complication were carried out by utilizing molecular dynamics. Conformational changes in metal binding for ligands were monitored by molecular dynamic computation and potential of mean force (PMF) using the method of the free energy perturbation. The microcystin-metal binding PMF simulation results exhibit that microcystin can have very stable binding free energy of -10.95 kcal/mol by adopting the Mg^{2+} ion at broad geometrical distribution of 0.5~4.5 Å, and show that the K^{+} ion can form a stable metal complex rather than other monovalent alkali metal ions

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL2.O-42

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:43, Chair: Sang Yun Han

Feasibility of 3-Phase direct immersion in-tube microextraction comparison with Single drop microextraction coupled with capillary electrophoresis

ji eun choi, Doo Soo Chung*

Division of Chemistry, Seoul National University, Korea

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME using commercial kits, LPME usually require more manual maneuvers. To overcome such shortcomings of LPME, we developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease using a commercial CE instrument. Here, we demonstrate direct immersion (DI)-ITME in a 3-phase configuration to enrich acidic compounds from an acidified aqueous sample to a basic acceptor plug through a thin organic phase. The feasibility and drawback of DI-ITME were investigated in comparison with direct immersion single drop microextraction (DI-SDME). Due to the lack of a hanging drop used in DI-SDME, DI-ITME is a quite simple and robust extraction method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL2.O-43

Area: Oral Presentation of Young Analytical Chemists II

Type: Oral Presentation, Time: FRI 10:45, Chair: Sang Yun Han

Investigation on The Stability of Uric Acid and Its Isotope (1,3-15N2) in Ammonium Hydroxide for The Absolute Quantification of Uric Acid in Human Serum

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In clinical diagnosis, it's well known that the abnormal level of uric acid (UA) in human body is implicated in diverse human diseases, for instance, chronic heart failure, gouty arthritis, diabetes, chronic renal failure, and kidney stones). In order to accurately diagnose UA-related diseases, the development of the method for the absolute quantification of UA in biological sample is required. As a primary method, an isotope dilution mass spectrometry (IDMS) has been used to obtain the accurate quantity of UA in blood or serum and also develop the certificated reference material (CRM) so as to provide a SI-traceability to clinical laboratories. Due to the low solubility of UA in water, an ammonium hydroxide (NH₄OH) has been considered as a promising solvent to increase the solubility of UA and prepare both UA and its isotope standard solution for next IDMS-based absolute quantification. But, because of using this NH₄OH solvent, it gives rise to the unwanted degradation of UA. In this study, we sought to optimize condition for the stability of UA in NH₄OH solution by varying the mole ratios of UA to NH₄OH at five different mole ratios of 1/1, 1/1.5, 1/2, 1/3, and 1/5.6, followed by LC-ID-MRM analysis. In addition, we also inspected minutely the effect of the storage temperatures [-20 °C and room temperature (RT)]. Finally, we performed the quantitative analysis of UA containing the KRISS serum certificated reference material (CRM, 111-01-02A) with diverse mixing ratios of UA to NH₄OH and then compared those values to its certification value.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-1**

Area: Oral Presentations of Young Scholars in Organic Division

Type: Oral Presentation, Time: THU 09:00, Chair: Cheol-Hong Cheon

Introduction of a New Hydroxybenzyne Precursors Induced by 1,3-Brook Rearrangement

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

Benzynes are highly strained and reactive alkynes and derived from an aromatic ring by removal of two ortho substituents. Because it has great activity and usefulness, a lot of attempt to make benzyne formation have been reported and especially, the method using silyaryl triflate in the presence of fluoride source has been employed. Herein, we report the design, synthesis and achievements of a new type of benzyne precursor which is capable of highly reactive benzyne intermediate induced by 1,3-silyl group migration on the aryl moiety. We would use this base-promoted benzyne generation method for the nucleophilic addition reaction and cycloaddition reaction and obtained meta-regioselective compounds in good to excellent yields. We also investigated plausible mechanism through previous reported method and crossover experiment.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-2**

Area: Oral Presentations of Young Scholars in Organic Division

Type: Oral Presentation, Time: THU 09:15, Chair: Cheol-Hong Cheon

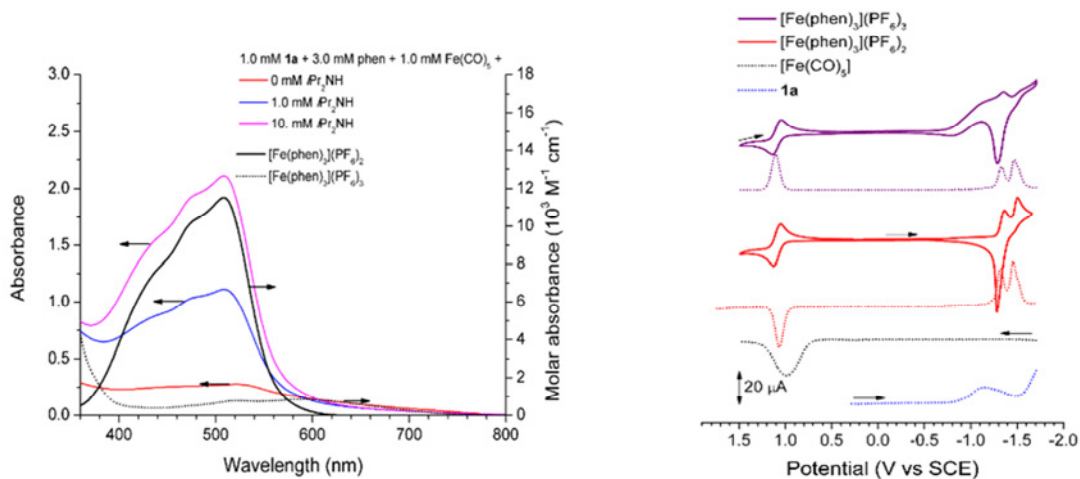
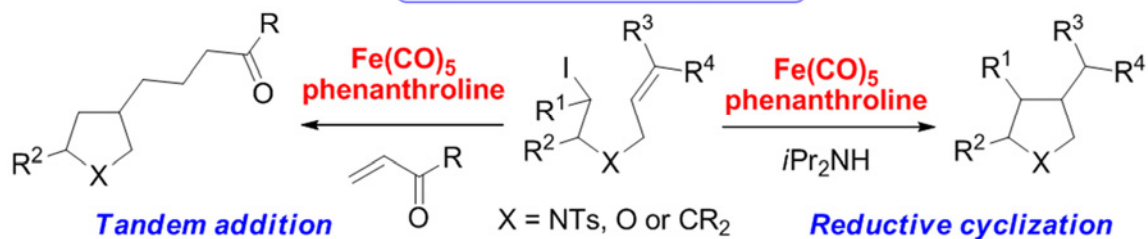
Single electron transfer strategy for reductive cyclization and oxidative cycloaddition reactions using iron polypyridyl complexes

Joon Young Hwang, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Reductive radical cyclization using low-valent iron pentacarbonyl [Fe(CO)₅] to generate radical species from alkyl iodides was achieved. A range of pyrrolidines, tetrahydrofurans, and carbocycles were synthesized via 5-*exo* cyclization reactions of alkyl radical intermediates generated by electron transfer from a system involving Fe(CO)₅, 1,10-phenanthroline, and diisopropylamine. In addition, we have successfully applied to the tandem radical reactions with Michael acceptor. We have found the presence of Fe²⁺(phen)₃ species during the reaction through UV-vis absorption spectroscopy and electrospray ionization mass spectrometry (ESI-MS), which are the distinct evidence that Fe and phenanthroline system acts as electron donor agents. Moreover, we have proved that radical pathway is main route by the radical clock reaction, TEMPO experiment, and electron paramagnetic resonance (EPR) studies to investigate iron(III) complex and phenanthroline radical anion species. Especially, iron(III) polypyridyl complexes can be used as single-electron oxidants with tertiary amines or anilines [$E_{ox} = 0.8-1.0$ V] for formation amine radical cation as a hydrogen atom source. In this regard, we planned oxidative reaction of tertiary amines with iron polypyridyl complexes. 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, we present reductive radical cyclization of iodoalkene and oxidative cycloaddition of tertiary amines with maleimides under mild reaction condition.

Radical generation via SET



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-3**

Area: Oral Presentations of Young Scholars in Organic Division

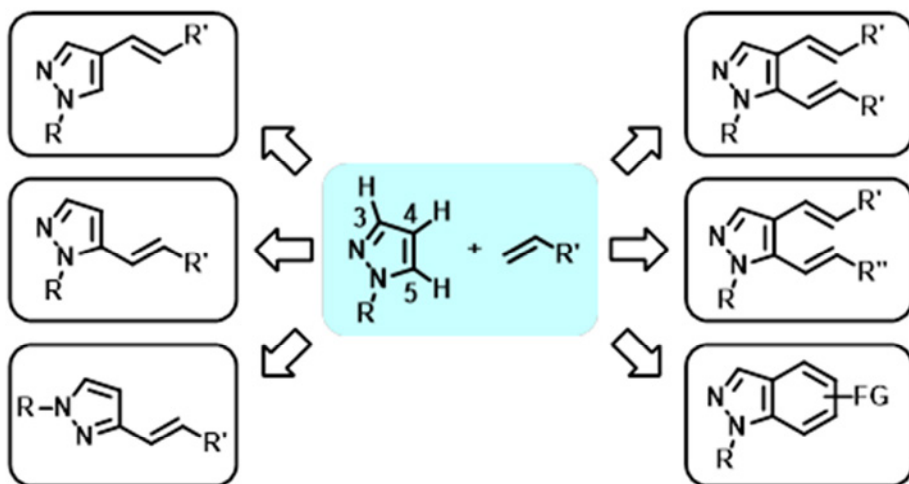
Type: Oral Presentation, Time: THU 09:30, Chair: Cheol-Hong Cheon

Pd-catalyzed Regioselective C–H Alkenylation of Pyrazoles

HyunTae Kim, Jung Min Joo*

Department of Chemistry, Pusan National University, Korea

We have developed Pd-catalyzed regioselective C4-, C5-, and di-alkenylation of pyrazoles. Kinetic isotope effects and H/D exchange experiments were performed in order to obtain mechanistic insights into C4- and C5-alkenylation. These Pd-catalyzed protocols gave a wide range of alkenylated pyrazoles from readily available, inexpensive pyrazoles and alkenes. In addition, thermal 6 π -electrocyclization and oxidation via dialkenylated pyrazoles provided functionalized indazoles, which have important roles in medicinal chemistry and material science. Furthermore, C5-alkenyl pyrazoles were useful for the preparation of 3-alkenyl pyrazoles that are not easily accessible by C–H alkenylation. This comprehensive strategy can provide a variety of pyrazole and indazole derivatives for applications in the development of biologically active compounds and functional materials.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-4**

Area: Oral Presentations of Young Scholars in Organic Division

Type: Oral Presentation, Time: THU 09:45, Chair: Cheol-Hong Cheon

Coupling between CO₂ and Epoxides Catalyzed by Fe(III) and Al(III) Complexes

Yuseop Lee, Kim Hyunwoo *

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

Carbon dioxide (CO₂) is one of fascinating C1 sources because it is cheap, abundant, and renewable. Moreover, CO₂ is relatively nontoxic compared to carbon monoxide or formaldehyde. Therefore, various kinds of CO₂ utilization methods have been developed not only because of these prominent features but also worldwide concerns of global warming. One of the promising CO₂ utilization methods is coupling reaction between epoxide and CO₂ to produce poly- or cyclic carbonate. Among several organometallic catalysts reported to date, the tripodal ligand based catalysts showed remarkable activity in the cyclic carbonate synthesis. According to the DFT computation, authors proposed a transition state where two oxygen atoms each from epoxide and CO₂ bind to the metal center in a cis fashion, thereby greatly lowering the activation barrier. Thus, highly active and selective catalysts for the coupling reaction of epoxide and CO₂ can be developed. In this context, we have designed a new class of N₁O₃ ligand which can combine epoxide and CO₂ into cyclic carbonate and polycarbonate respectively. In this presentation, we will introduce highly efficient and selective Fe(III)-N₁O₃ complexes for the selective synthesis of cyclic carbonate. We will also demonstrate that Al(III)-N₁O₃ complexes can be used for selective synthesis of polycarbonates and chemoselective conversion of epoxy amines into amino carbonates or hydroxyl oxazolidinones.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-5**

Area: Oral Presentations of Young Scholars in Organic Division

Type: Oral Presentation, Time: THU 10:00, Chair: Cheol-Hong Cheon

A tandem radical cyclization route to pleuromutilin core structure and unusual ring closure mechanism

Rira Kim, hee-yoon lee*

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

The tricyclic diterpene fungal metabolite (+)-Pleuromutilin was isolated in 1951 by Kavanagh and co-workers from several species of basidiomycetes and has been found noteworthy for antibacterial activity through a novel mode of action involving binding to the prokaryotic ribosome.¹ With the promising effect against the resistant bacteria to antibiotics due to its unique mechanism of action, its intricate skeleton including rare 8-membered ring of tricyclo-[5.4.3.01,8]-tetradecane has intrigued the synthetic chemistry community. To construct the interesting tricyclic framework of pleuromutilin, there have been various approaches. We have reported previously the total synthesis of subermosene with tricyclo-[4.3.2.01,5]-undecane via vinyl radical tandem cyclization from the cyclopentene containing appropriate dibutylene tethers.² Furthermore, the tendency of cyclization were also shown with larger ring system from 5- to 8-membered ring.³ Based on those results, we envisioned that the core structure of pleuromutilin would be obtained in one-pot from cyclooctene with requisite dibutylene tethers in similar way. Along the way, we observed unusual ring closure by radical rearrangement derived from steric and conformational factors. In this presentation we will discuss the mechanism of the reaction and eventual construction of the framework of pleuromutilin consisting of tricyclo-[5.4.3.01,8]-tetradecane. References 1. (a) Hogenauer, G. Eur. J. Biochem. 1975, 52, 93, (b) Tang, Y. Z.; Liu, Y. H.; Chen, J. X. Mini-Rev. Med. Chem., 2012, 12, 53. (c) Kirst, H. A. Expert Opin. Ther. Pat., 2012, 22, 15. 2. Lee, H. Y.; Kim, B. G. Org. Lett. 2000, 2, 19513. Lee, H.-Y.; Lee, S.; Kim, B. G.; Bahn, J. S. Tetrahedron Lett. 2004, 45, 7225

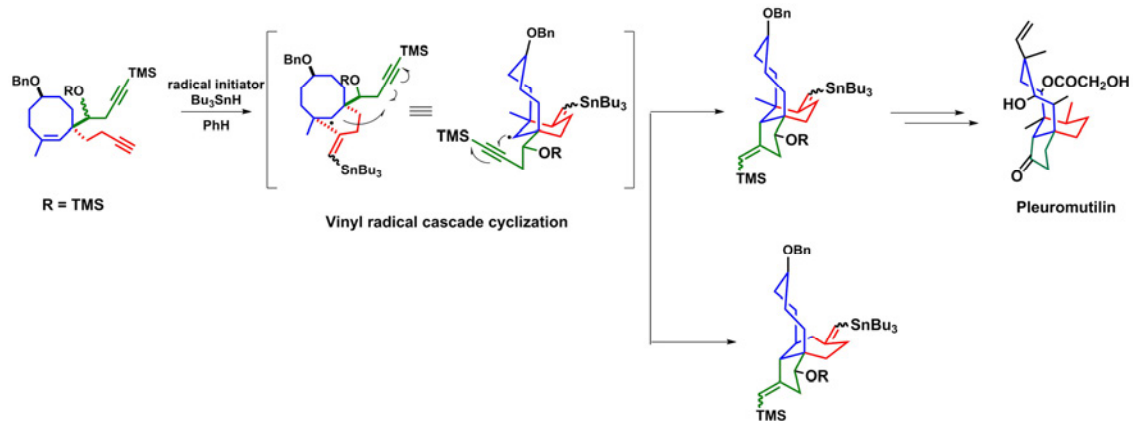


Figure 1. Vinyl radical cascade cyclization toward tricyclic skeleton of pleuromutilin.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-6**

Area: Oral Presentations of Young Scholars in Organic Division

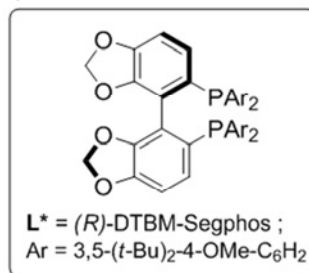
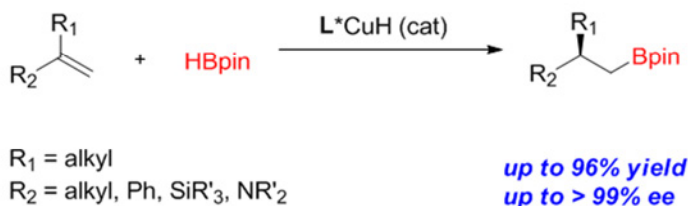
Type: Oral Presentation, Time: THU 10:15, Chair: Cheol-Hong Cheon

Enantioselective Hydroboration of 1,1-Dialkylsubstituted Alkenes by Copper Catalysis

Won Jun Jang, Seung Min Song, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Highly enantioselective hydroboration method of 1,1-disubstituted alkenes has been developed. This reaction provides an efficient synthetic method of enantioenriched β -borylalkanes. In the presence of DTBM-Segphos-ligated Cu catalyst, a range of 1,1-disubstituted alkenes with an alkyl, aryl, silyl, amine substituent produced alkylboron compounds in good yields and excellent enantioselectivities up to 99% ee. Furthermore, catalyst loading as low as 1 mol% could be furnished desired product without decrease of yield and selectivity.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-7**

Area: Oral Presentations of Young Scholars in Organic Division

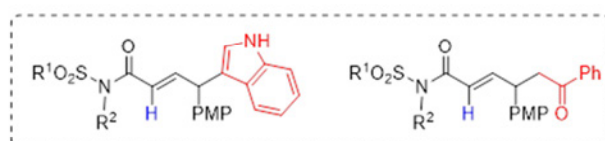
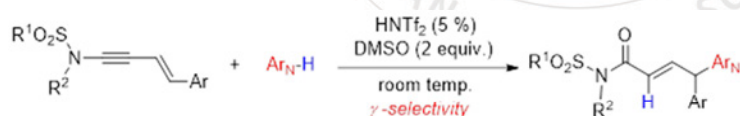
Type: Oral Presentation, Time: THU 10:30, Chair: Cheol-Hong Cheon

Umpolung Reactivity of Enyamides: Entry into Gamma-Substituted Carbonyl Compounds

Huong Quynh Nguyen, Seunghoon Shin^{*}

Department of Chemistry, Hanyang University, Korea

Recently, we have shown that the Brønsted acid-catalyzed reaction of ynamides displays a formal enolate umpolung reactivity, allowing substitution of various arene nucleophiles at the α -position of the carbonyls. Herein, we extended this method to enyamides and observed a good to excellent level of regioselectivity for the γ -substitution of the amides. Depending on the nucleophiles, unactivated indoles and silyl enol ethers participated as excellent nucleophiles, leading to γ -indolyl- α,β -unsaturated amides and 1,6-dicarbonyl compounds, respectively. Importantly, dimethyl sulfoxide could be used as innocuous and atom-efficient oxidants that can replace previously described pyridine-N-oxides.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.O-8**

Area: Oral Presentations of Young Scholars in Organic Division

Type: Oral Presentation, Time: THU 10:45, Chair: Cheol-Hong Cheon

Total Synthesis of α -Amanitin Derivative: A Novel Cytotoxic Agent for Antibody Drug Conjugate Payload

**Gangadhar Rao Mathi, Jong Yeon Hwang, jae du ha¹, Chang-Soo Yun, Sung Yun Cho¹,
Hyoung Rae Kim¹, PILHO KIM^{*}**

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

¹*WCI, Korea Research Institute of Chemical Technology, Korea*

α -Amanitin belongs to a large group of protoplasmic mushroom toxins known as amatoxin family isolated from the green death cap mushroom *Amanita phalloides*. α -Amanitin is characterized by a defined rigid structure consisting of a bicyclic octapeptide, with an intraannular linkage known as a tryptathionine bridge between tryptophan and cysteine. The toxin shows remarkable binding affinity for eukaryotic RNA polymerase II. Inhibition of RNA polymerase II compromises cellular homeostasis and leads to apoptosis. Amatoxins are usually isolated from collected *amanita phalloides* mushrooms or from pure cultures. However the amounts that can be obtained are rather low and the flexibility for further modifications are limited. The use of entirely synthetic routes to amatoxins may offer the supply of large quantities required for therapeutic use. No fully solution phase synthetic approach to the relevant amatoxins has been reported so far. Hence there is high need in the prior art to identify alternate method for synthesizing α -Amanitin and its derivatives. α -Amanitin seems to be a suitable toxic payload for use in an Antibody-Drug Conjugate (ADC) because of the unique mode of action and the molecular characteristics of the toxin. A new α -Amanitin derivative applicable for diverse linker chemistry was designed to improve stability with prolonged cytotoxicity. Retrosynthesis and the utilization of orthogonal protecting groups during the course of total chemical synthesis of α -Amanitin derivative will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-8**

Area: Oral Presentation of Young Material Chemists

Type: Award Lecture in Division, Time: THU 10:20, Chair: Myung-Gil Kim

Unconventional Approaches for Energy Applications

Min Hyung Lee

Department of Applied Chemistry, Kyung Hee University, Korea

In many research fields, researchers are often stuck with problems that are difficult to overcome for decades although tremendous effort has been devoted. Finding high-performance catalysts and photoelectrochemical (PEC) electrodes for water splitting and CO² reduction is the one of great examples. We might be able to find solutions from unconventional routes. In this talk, I will introduce some examples of unconventional approaches that can potentially provide solutions in sluggish research fields. First, enhanced water oxidation can be achieved by inducing spontaneous dipoles in PEC electrodes compared to those without dipoles. Second, well-designed nanopatterned array structures can drastically improve the selectivity of electrochemical conversion of water and CO₂. Lastly, simple surface chemical functionalization can change triboelectric property of a polymer substrates and can enhance power output of nanogenerators compared to conventional engineering methods.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.O-1**

Area: Oral Presentation of Young Material Chemists

Type: Oral Presentation, Time: THU 09:00, Chair: Myung-Gil Kim

Direct Writing of Molecular Junction Achieved by in situ Encapsulation of Liquid Metal Microelectrode with Photo-curable Polymers

Seo Eun Byeon, Kim Miso, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Difficulty in forming geometrically well-defined, non-invasive and compliant electrical contact over molecular monolayers makes it challenging to achieve molecular-scale electronic devices that function in high yields and with good reproducibility. Moreover, none of previously reported methods to form organic-electrode contacts at nano- and micrometer scales demonstrated directly addressable contacts in an untethered form in ambient conditions without using cumbersome equipment and nanolithography. Here, we show that in situ encapsulation of liquid metal (eutectic Ga-In) microelectrode with a convenient photo-curable polymeric scaffold enables direct writing of high-yielding molecular junctions on self-assembled monolayers in ambient conditions. The formed junctions function in quantitative yields and afford tunneling currents with high reproducibility as well as low temperatures and bent conditions. Furthermore, the low wettability of polymeric scaffold brings about water-proof effect for junction measurements in aqueous environment. The results reported here promise a massively parallel printing technology for constructing integrated circuits based on individual molecules as an active electronic component.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-2**

Area: Oral Presentation of Young Material Chemists

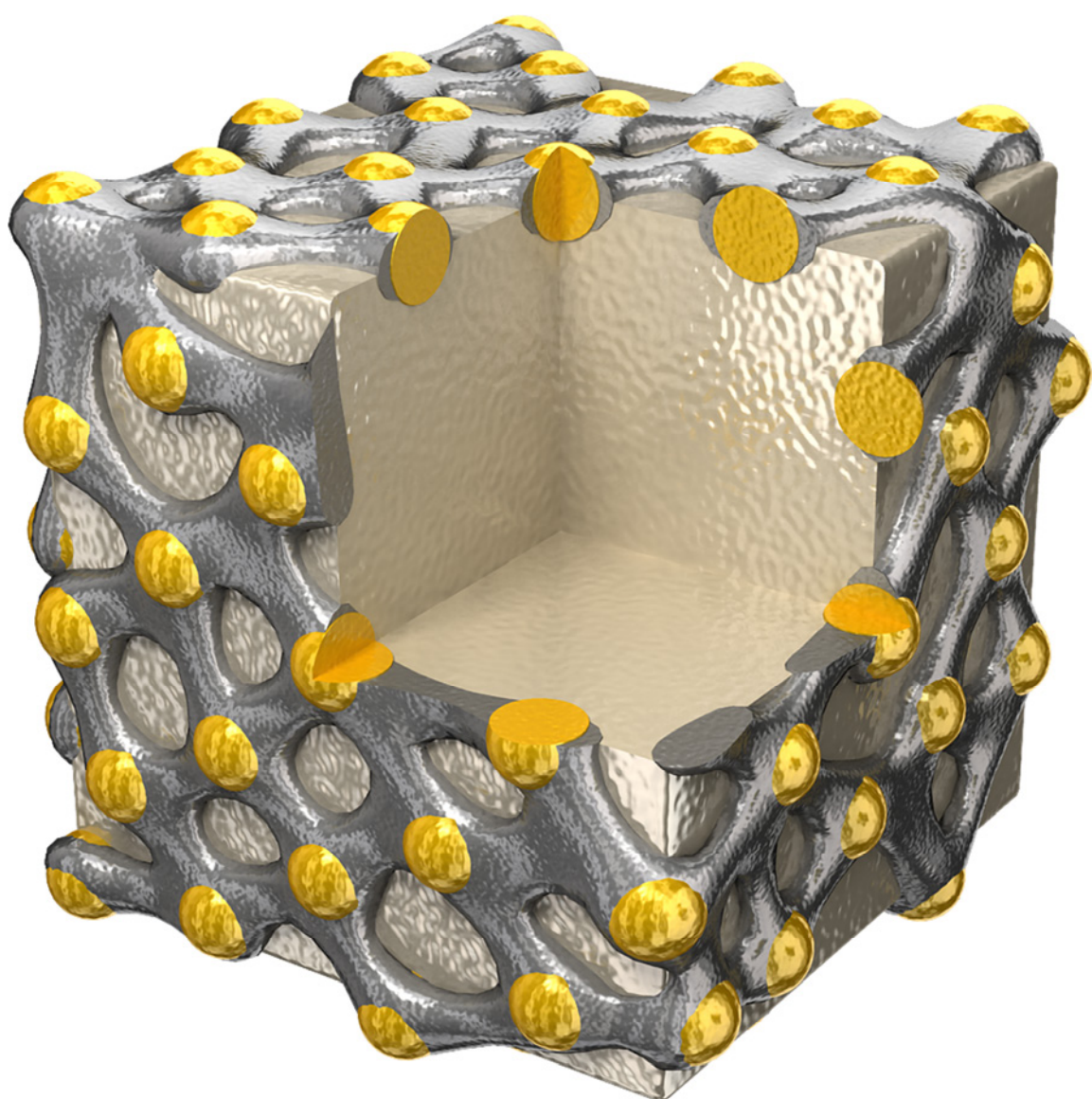
Type: Oral Presentation, Time: THU 09:10, Chair: Myung-Gil Kim

Synthesis of nanocubic photocatalysts composed of gold, silver and silver chloride using semi-sacrificial templates

Jang Ho Joo, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

We synthesized AgCl/Au/Ag composite nanocubes (AgCl/Au/AgNCs) which consist of the core-AgCl nanocube (AgCINC) surrounded by 'in-panel' Au nanoparticles and continuous Ag matrix. In comparison to the polyol synthesis, the aqueous synthesis of AgCINCs using HAuCl₄, AgNO₃, and polyvinylpyrrolidone is advantageous because it is fast and reliable. As-synthesized AgCINCs were combined with ascorbic acid to co-reduce the remaining AuCl₄⁻, Ag⁺ and AgCINCs. After the co-reduction, NH₄OH was used to confirm the reduced nanostructures by eliminating the AgCINCs that still existed in the AgCl/Au/AgNCs. Consequently, we obtained hollow nanoboxes whose panels are composed of discontinuous Au nanoparticles in continuous Ag mesh matrix (Au#AgNBs). In order to investigate the chemical components of the three nanostructures, X-ray powder diffraction (XRD) patterns were obtained for the AgCINCs, the AgCl/Au/AgNCs, and the Au#AgNBs, which clearly showed the formation of AgCINCs, the reduction of metallic precursors to form the AgCl/Au/AgNCs, and the removal of AgCINCs to leave only the Au#AgNBs. The distribution of Au and Ag in the panel of the AgCl/Au/AgNC was analyzed after the elimination of the AgCINCs by energy-dispersive X-ray spectroscopy (EDX). Importantly, the EDX results demonstrated that the panels of the AgCl/Au/AgNCs were not atomically alloyed structures, but composed of small Au nanoparticles and Ag mesh matrix. In addition, we investigated the catalytic properties of the AgCINCs, the AgCl/Au/AgNCs and the Au#AgNBs for the oxidation of o-phenylenediamine (OPD) to 2,3-diaminophenazine (DPA). The AgCl/Au/AgNCs exhibited the highest catalytic activity than AgCINCs and Au#AgNBs demonstrating the importance of the co-existence of Au, Ag and AgCl for the catalytic properties.



AMERICAN CHEMICAL SOCIETY

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-3**

Area: Oral Presentation of Young Material Chemists

Type: Oral Presentation, Time: THU 09:20, Chair: Myung-Gil Kim

Morphology Tunable Hybrid Carbon Nanomaterials with Solvatochromism

Yuri Choi, Byeong-Su Kim*

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

The tunable photoluminescence of carbon-based nanomaterials has received much attention for a wide range of applications. Herein, we report a unique, broad-solvatochromic hybrid carbon nanosheet (CNS) synthesized through the hydrothermal carbonization of molecular precursors exploiting graphene oxide as a template, resulting in the formation of clusters of carbon nanorings on the surface of graphene-oxide nanosheets. Under UV and visible-light excitation, the hybrid CNS exhibited tunable emission spanning the wide range of colors in a series of solvents with different polarities. This interesting spectroscopic behavior was found to originate from hydrogen-bonding interactions between CNS and solvents, which eventually induced the morphological transition of CNS from 2-dimensional sheets to 3-dimensional crumpled morphologies affecting the lifetimes of emissive states. This novel carbon nanostructure may open up a new possibility in tailoring the photophysical properties of carbon nanomaterials.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.O-4**

Area: Oral Presentation of Young Material Chemists

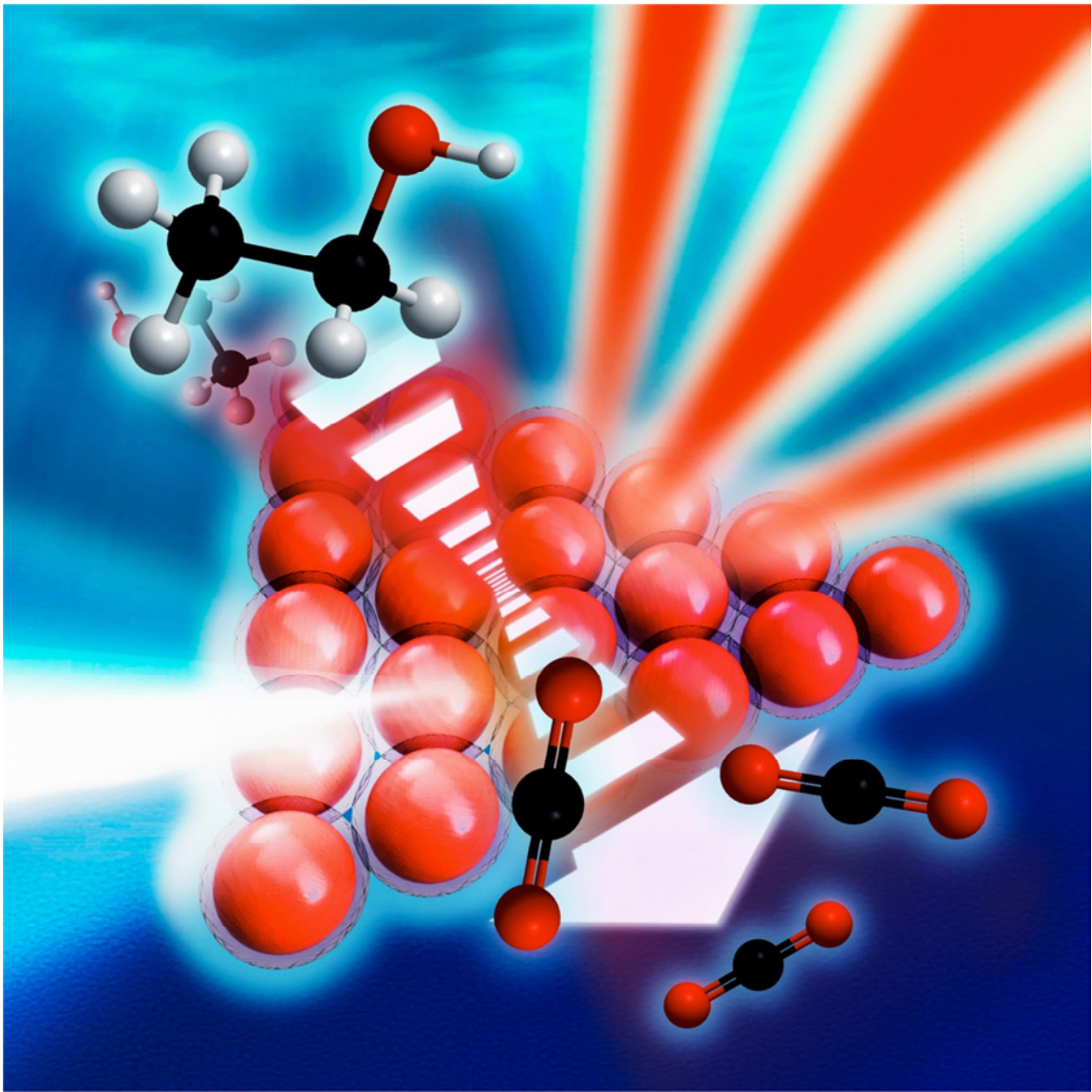
Type: Oral Presentation, Time: THU 09:30, Chair: Myung-Gil Kim

Core-Shell Nanoparticle Clusters with Integrated Plasmonic and Catalytic Functions

Seunghoon Lee, Sang Woo Han*

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

A new synthetic strategy for the preparation of colloidal clusters of core-shell nanoparticles with plasmonic cores and catalytically active shells is reported. The Au@M (M = Pd or Pt) nanoparticle clusters (NPCs) with a high density of sub-1 nm interparticle gaps were successfully prepared by the deposition of Pd or Pt shells onto thermally activated Au NPCs. The prepared Au@M NPCs showed remarkably enhanced plasmonic performance compared to their Au@M nanoparticle counterparts, which can be attributed to the localization of a strong electromagnetic field at the interparticle gaps. In situ real-time Raman spectroscopy and plasmon-enhanced electrocatalysis experiments demonstrated that the controlled assembly of core-shell nanoparticles is a very effective route for the synergistic integration of plasmonic and catalytic functions in a single platform.



AMERICAN CHEMICAL SOCIETY

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-5**

Area: Oral Presentation of Young Material Chemists

Type: Oral Presentation, Time: THU 09:40, Chair: Myung-Gil Kim

Gyromagnetic Plasmonic Nanorods for Shear Force-Induced Biosensing

Insub Jung, Sungho Park^{1,*}

Department of Energy Science, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

Biosensing based on the localized surface plasmon resonance of metallic nanostructures is a powerful tool for the detection of target species. To increase sensitivity, the systematic synthesis of complex nanostructures along with the design of a sensing platform with a rational configuration is critically important. However, most LSPR-based sensors operate in a passive and static way, hindering further improvements to their sensitivity and detection time. Herein, we report an unprecedented active and dynamic sensing platform based on a LSPR configuration that is modulated by using an external magnetic field. Electrochemically-synthesized Au/Fe/Au nanorods exhibited plasmonically-active behavior through plasmonic coupling, and the middle ferromagnetic Fe block responded to a magnetic impetus, allowing the nanorods to be modulated. The shear force variation induced by the specific binding events between antigens and antibodies on the nanorod surface is used to enhance the sensitivity of detection of antigens in the plasmonics-based sensor application. As a proof-of-concept, influenza A virus (HA1) was used as a target protein. This conceptual sensing method provides a new platform for active plasmonic-magnetic biosensing.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-6**

Area: Oral Presentation of Young Material Chemists

Type: Oral Presentation, Time: THU 09:50, Chair: Myung-Gil Kim

Magnesium Silicide Utilized as a Reactive Precursor for the Facile Synthesis of Silicon-Based Composite Electrodes for Lithium-Ion Batteries

Min seok Kang, Won Cheol Yoo*

Department of Applied Chemistry, Hanyang University, Korea

Recently, it has been clearly elucidated that nanostructured Si-based composites hybridized with protective and conductive materials can present enhanced electrochemical performance as anodes for Li-ion batteries (LIBs). One of remaining issues is to develop a sustainable and economic method to synthesize these composites on a large scale for industrial applications. Herein, we introduce a modified magnesiothermic reaction route to prepare the aforementioned Si-based composite electrodes using sea-sand derived Mg_2Si as a reactive precursor. Owing to its reducibility and lability, Mg_2Si can readily reduce group IVA oxides, such as Na_2CO_3 , SiO_2 , GeO_2 , and SnO_2 , resulting in macroporous Si surrounded by the reduced forms of the counter reactants (C, Si, Ge, and Sn, respectively), some of which can be electrochemically attractive. Notably, the porous Si-based composite can be synthesized by a simple solid state reaction, so simplicity and scalability can be obtained. Also, the sea sand precursor is naturally-abundant; hence this process can be cost-effective, scalable, and sustainable. Porous Si@C composite can be synthesized from the modified magnesiothermic reaction using a sea sand-derived Mg_2Si precursor, showing a specific capacity of 1000 mAh/g at 200th cycle. Potentially this process can be used for practical synthesis of Si-based composites.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.O-7**

Area: Oral Presentation of Young Material Chemists

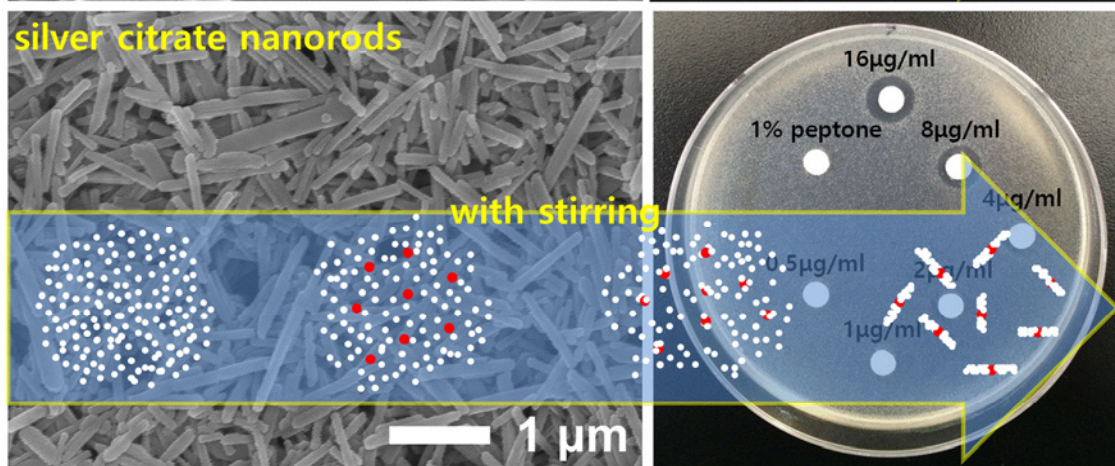
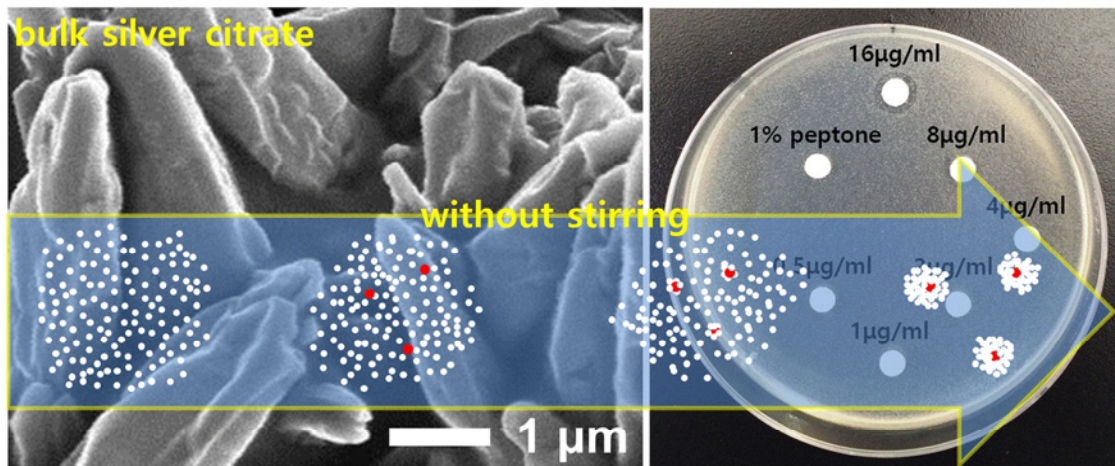
Type: Oral Presentation, Time: THU 10:00, Chair: Myung-Gil Kim

Asymmetric Growth of Silver Citrate Compounds by Mechanical Stirring and Their Enhanced Antimicrobial Activity

Jong Kuk Lim

Department of Chemistry, Chosun University, Korea

The development of a new class of antibiotics is urgently needed, because antibiotic resistance became a serious problem in the pharmaceutical and medical fields. Recently, silver compounds, composed of silver and organic molecules, have been developed as effective antimicrobial agents. For instance, silver citrate ($\text{Ag}_3\text{C}_6\text{H}_5\text{O}_7$; Ag-Cit) compounds prepared in the form of precipitates can exhibit a strong antimicrobial activity. Ag-Cit compounds were easily prepared in the mixture of AgNO_3 and trisodium citrate dihydrate ($\text{C}_6\text{H}_5\text{Na}_3\text{O}_7 \cdot 2\text{H}_2\text{O}$) solutions. Herein, we demonstrated that simple mechanical stirring significantly changed the morphology (shape and size) of Ag-Cit from bulk (bulk Ag-Cit) to rod-like nanostructures (Ag-Cit nanorods). Ag-Cit nanorods exhibited antimicrobial activity stronger than that of bulk Ag-Cit against both Gram-negative and -positive bacteria. These data indicate that the bactericidal activity of Ag-Cit compounds is dependent on their morphology and will provide valuable information for the development of antimicrobial materials based on Ag-Cit compounds.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.O-7**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Award Lecture in Division, Time: THU 10:30, Chair: JinHo Jang

Electrochemistry of Metal Nanoclusters

Dongil Lee

Department of Chemistry, Yonsei University, Korea

Metal nanoclusters containing a few to a few hundreds of metal atoms have been the focus of recent investigations because of their novel electronic, optical, and catalytic properties. They appear to represent the bulk-to-molecule transition region where electronic band energetics yield to quantum confinement effects and discrete electronic states emerge. This presentation will highlight work from my group that reports the progress of the fundamental science and technological applications of these metal nanoclusters. Voltammetry of the metal nanoclusters displays unique redox peaks and size-dependent electrochemical HOMO-LUMO gaps that can be related with optical and calculated energy gaps. These nanoclusters also show excellent electrocatalytic activity toward oxidation of biologically relevant analytes such as dopamine and glucose, which has practical implications in amperometric sensing. In addition, doped metal nanoclusters opened an avenue to tune their electronic properties and redox potentials for the development of tailored electrocatalysts for hydrogen evolution and CO₂ reduction reactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.O-1**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 09:00, Chair: JinHo Jang

Electrocatalytic Hydrogen Production on Molecular-like Metal Nanoclusters

woojun choi, Kyuju Kwak, Minseok Kim, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Hydrogen has received great attention with respect to its possibility for replacing fossil fuel as alternative energy sources. Hydrogen evolution reaction (HER) catalysts are usually divided into two categories such as metallic heterogeneous catalysts and synthetic molecular homogeneous catalysts. The latter usually mimicking neutral enzyme, hydrogenase, that is one of the most active HER catalyst due to its unique proton relaying process and thermodynamically neutral Gibbs free energy for binding between H^+ and active site ($\Delta G_H = \sim 0$ eV). Ultrasmall Au_{25} nanocluster that has both metallic and molecular-like characteristics exhibits distinctive electrochemical properties and unique catalytic activities. In this presentation, we report electronic structures and catalytic properties of $Au_{25}(SR)_{18}$ and bimetallic $PtAu_{24}(SR)_{18}$ nanoclusters (SR = thiolate). Electrocatalytic HER activities of nanoclusters were demonstrated by linear sweep voltammetry (LSV) and controlled potential electrolysis (CPE) was conducted for real gas detection. Calculated ΔG_H by density functional theory (DFT) supported the intrinsic HER activities of nanoclusters. Au_{25} catalyzes hydrogen production with onset potential (E_{onset}) = -0.3 V vs. RHE and turnover frequency (TOF) for HER reached $8.8 s^{-1}$ at -0.6 V. $PtAu_{24}$ showed promoted HER activity with very low E_{onset} (70 mV) that is comparable to that of hydrogenase (~ 100 mV) and high TOF ($33.4 s^{-1}$ at -0.6 V). This would be ascribed that moderate ΔG_H of $PtAu_{24}$ (-0.059 eV) compare to Au_{25} that have too weak binding energy with H^+ ($\Delta G_H = 0.539$ eV).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.O-2**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 09:15, Chair: JinHo Jang

Electrochemical Detection of Dopamine using Conducting Polymer/ SrMoO₄ Composite

mahmood hassan akhtar, abhijit pandurang jadhav, Yoon Bo Shim*

Department of Chemistry, Pusan National University, Korea

A highly sensitive and selective dopamine sensor was prepared by conducting polymer/ metal oxide composite. Highly crystalline and spherical shaped strontium molybdate nanostructures were prepared by conventional hydrothermal method using poly(diallyldimethylammonium chloride) as a surfactant. The conducting polymer, TTBA (3'-(p-benzoic acid) - 2,2':5'2'' -terethiophene) / SrMoO₄ / Nafion was tested for the selective detection of dopamine. The electro-polymerized composite of conducting polymer /SrMoO₄ / Nafion was characterized by X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM). The glassy carbon electrode modified with conducting polymer/ SrMoO₄/ Nafion shows high stability and performance for longer time. The dopamine sensor showed a wide dynamic range of 50 nM ~ 2 mM with a detection limit of 20 nM. The proposed sensor exhibited a high selectivity towards the detection of dopamine in the presence of different biological interferences.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ELEC.O-3

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 09:30, Chair: JinHo Jang

Effect of two dopants on the electronic structure of $M_2Au_{36}(SC_6H_{13})_{24}$ ($M=Pt, Pd$)

Minseok Kim, Dongil Lee^{*}, Kyuju Kwak

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 a 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 excellent stability and different optical and electrochemical properties. In this presentation, we report the optical and electrochemical characteristics of 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 gap between highest occupied molecular orbital-lowest unoccupied molecular orbitals 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 having 12 superatomic electron exhibits remarkably different optical and electrochemical properties from those of the 14 electron cluster systems such as $[Au_{38}(SR)_{24}]^0$ and $[Pt_2Au_{36}(SR)_{24}]^{2-}$.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.O-4**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 09:45, Chair: JinHo Jang

Iridium-Iridium Oxide Nanofibers as an Improved Electrocatalyst for Hydrogen Evolution Reaction

Su-jin Kim, Myung Hwa Kim¹, Chongmok Lee, Youngmi Lee*

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

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

Hydrogen evolution reaction (HER) has been actively studied for renewable electrochemical storage systems and energy conversion. HER electrocatalysts are required to have low overpotentials with generating high cathodic current densities of HER. Therefore, various materials have been developed and characterized as electrocatalysts for HER. In this research, we synthesize iridium-iridium oxide nanofibers (Ir-IrO₂ nanofibers) via simple electrospinning of an iridium precursor/polymer solution and subsequent calcination at various temperatures (300, 500, 700, and 900 °C). The structural morphologies and compositions of Ir-IrO₂ nanofibers calcined at various temperatures are characterized by field emission scanning electron microscopy, transmission electron microscopy and X-ray diffraction. When the calcination temperature is increased, the portion crystallized IrO₂ species is also increased, and Ir metal portion is decreased. The electrochemical HER activities of Ir-IrO₂ nanofibers are studied using rotating disk electrode linear sweep voltammetry. The onset potential, Tafel slope and stability for HER on synthesized Ir-IrO₂ nanofibers are compared with those on platinum. To understand the experimental results on the fundamental basis, HER catalyzed by Ir-IrO₂ nanofibers is studied using density functional theory calculations based on d-band theory. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2017R1A2A2A14001137).

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.O-5**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 10:00, Chair: JinHo Jang

Non-Grignard and Lewis acid-free sulfone electrolytes for rechargeable magnesium batteries

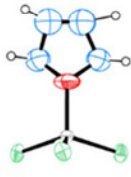
Sung-Jin Kang, Seung-Tae Hong, Hochun Lee*

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

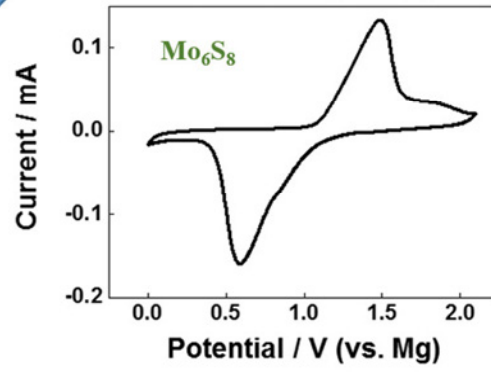
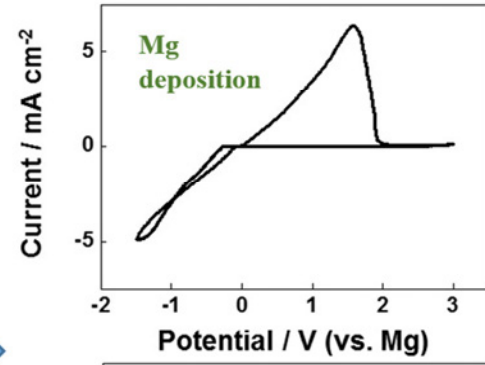
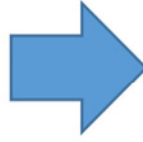
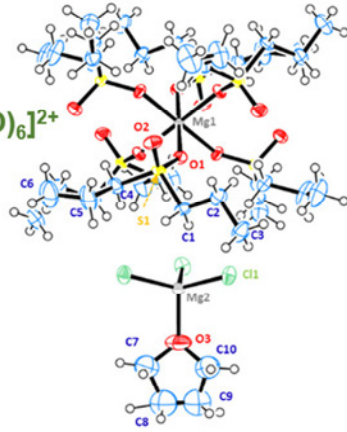
A major challenge for developing rechargeable Mg-ion batteries (MIB) is the lack of suitable electrolytes. We report herein dialkyl sulfones as non-Grignard and Lewis acid-free MIB electrolytes. In particular, a dipropyl sulfone (DPSO)/tetrahydrofuran (THF) (1/1, v/v) solution with MgCl_2 salt exhibits high ionic conductivity (1.1 mS cm^{-1} at 30°C), Mg cycling efficiency ($> 90\%$), and anodic stability (ca. 3.0 V vs Mg). As evidenced by single crystal X-ray diffraction analysis, a novel $[\text{Mg}(\text{DPSO})_6]^{2+}$ cation complex balanced by two $[\text{MgCl}_3(\text{THF})]^-$ anions is identified in the DPSO/THF solution. The DPSO/THF electrolyte also enables excellent cycle performance (> 300 cycles) of a Chevrel phase Mo_6S_8 cathode and displays a decent compatibility with an organic cathode (3,4,9,10-perylenetetracarboxylic dianhydride, PTCDA). Along with the superior electrochemical properties of the DPSO/THF electrolyte, its innate chemical stability and eco-friendly nature make it a promising MIB electrolyte.

MgCl₂ DPSO/THF

[MgCl₃(THF)]⁻



[Mg(DPSO)₆]²⁺



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.O-6**

Area: Oral Presentation of Young Scholars in Electrochemistry

Type: Oral Presentation, Time: THU 10:15, Chair: JinHo Jang

The role of solid electrolyte interphase (SEI) on sodium metal in sodium-oxygen batteries

Younguk Jung, Hye Ryung Byon *

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

Metal-oxygen batteries have been paid attention to one of the promising next-generation batteries applied for electric vehicles, thanks to higher energy density than current lithium-ion batteries. However, instability of superoxide (O_2^-) formed through O_2 reduction severely incurs side reaction, which alleviates voltaic efficiency and cycling performance. The lithium-oxygen ($Li-O_2$) batteries typically show large charge overpotential and poor cycling stability. However, the superoxide species is more stable with larger size of alkaline metal ion, resulting in less side reactions, which has been demonstrated in the sodium-oxygen ($Na-O_2$) batteries. Nevertheless, poor cycling performance is still measured, which have not yet fully understood. Here we demonstrate one of the critical reasons for low cycling stability from Na metal as the negative electrode. We observed nanometer size of uneven precipitates that passivate the positive carbon nanotube electrode surface before and after galvanostatic tests. We attributed this unintended deposit to soluble solid electrolyte interphase (SEI) formed from the Na metal interphase, which is in line with depletion of Na metal after cycling. With increasing stability of SEI layer, the precipitate disappears from the carbon electrode surface and discharge overpotential is significantly reduced. In the presentation, I will discuss improving stability of SEI layer on Na metal and the correlated cycling result of $Na-O_2$ battery and Na metal condition in detail.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.O-1

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 09:00, Chair: Dongwook Kim

Electrocatalytic Hydrogen Production Using Ligand-Protected Metal Nanoclusters

Kyuju Kwak, woojun choi, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Hydrogen has been considered as an alternative energy carrier and generated the intense interest in creating catalytic systems that can efficiently produce hydrogen from water. Hydrogen evolution reaction (HER) has been studied with various catalysts such as bulk metals and metal complexes represented by Pt metal and hydrogenase. Ultra-small metal nanoclusters, especially molecular-like Au₂₅ nanoclusters that have similar characteristic with both bulk metals and metal complexes have distinctive catalytic activities. Furthermore, the activity for the catalytic reactions can be readily controlled by introducing a foreign metal such as Pt into the nanocluster platform or tuning the ligands with functional groups. In this presentation, we report that atomically engineered metal nanoclusters for example, Au₂₅(SR)₁₈ and PtAu₂₄(SR)₁₈ where SR is thiolate, can be effectively used as HER catalysts. First, mono Pt doped Au₂₅(SR)₁₈, PtAu₂₄(SR)₁₈, shows remarkable HER activity with very low onset-potential ($E_{\text{onset}} = 70$ mV vs. RHE) that is comparable to that of natural hydrogenase (~100 mV) enzymes. 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. Second, sulfonate ligands-protected PtAu₂₄(SR)₁₈ exhibits rate constant of 628,000 s⁻¹ in water at moderate overpotential (0.7 V); significantly higher than that reported to date for the highest active nickel complex (170,000 s⁻¹ at 0.47 V) catalysing hydrogen formation with pendant amines. The functional group of the thiolate ligands is particularly effective in increasing the accessibility of proton, most likely facilitated by proton relay effect between solvent to active-site. These results highlight the importance of metal core and ligand engineering as an indispensable tool in the rational design of metal nanoclusters, which can improve the catalytic properties of nanocluster catalysts.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.O-2

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 09:15, Chair: Dongwook Kim

Free Standing Blue TiO₂ Nanotube Arrays on Transparent Conductive Oxide Electrodes for High-Efficiency Solar Water Splitting

Hye Won Jeong, Byeong-ju Kim, Hyunwoong Park*

School of Energy Engineering, Kyungpook National University, Korea

Free-standing, one-dimensional TiO₂ nanotube arrays (TNAs) with disordered surface structure are synthesized on transparent conducting substrates, and their opto-physicochemical properties and photoelectrocatalytic (PEC) performances are examined in detail. TNAs grown on titanium foils are transplanted onto fluorine-doped SnO₂ substrates via a two-step anodization process (denoted W-TNAs), followed by being reduced electrochemically for 20 and 90 s (denoted B-TNAs-20 and 90, respectively). As-transplanted W-TNAs exhibit the low PEC activities in terms of photocurrent, and oxygen evolution reaction (OER), and oxidations of inorganic and organic substrates (iodide and urea, respectively) under simulated sunlight (AM 1.5; 100 mW·cm⁻²) primarily because of sluggish charge transfers through low electrical conductive TNAs framework. The quick electrochemical reduction of W-TNAs leads to 8-fold larger photocurrent, while significantly accelerating the OER by three times, and the oxidations of iodide and urea by 2 and ~20 times, respectively. Such enhanced PEC activity of B-TNAs is attributed to creation of Ti³⁺ and associated oxygen vacancy (examined with XPS, EPR, and Raman), strengthening n-type character and thereby increasing electrical conductivity (examined with Mott-Schottky and Nyquist). Time-resolved photoluminescence spectra further reveal that the lifetime (τ) of photogenerated charge carriers in B-TNAs ($\tau = 0.33$ ns) is an order of magnitude shorter than that of W-TNAs ($\tau = 3.63$ ns). The disordered surface exhibits lower Faradaic efficiency for multi-electron transferred oxidation reactions whereas higher Faradaic efficiency for single-electron transfer oxidations compared to W-TNAs. Detailed surface characterization and PEC mechanism are discussed. This work was financially supported by the Korea Ministry of Environment as Waste to Energy-Recycling Human Resource Development Project (YL-WE-17-001), Space Core Technology Development Program (NRF-2014MA3A3A02034875), and Nano-Material Technology Development Program (NRF-2016M3A7B4908169).

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ENVR.O-3

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 09:30, Chair: Dongwook Kim

Heterojunction p-n-p Cu₂O/S-TiO₂/CuO: Synthesis and application to photocatalytic conversion of CO₂ to methane

HyeRim Kim, SU IL IN*

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

Photocatalytic conversion of CO₂ to fuel is a topic of great current interest. The problem is a challenging one, requiring a photocorrosion-stable, industrially-scalable, broad-spectrum light absorbing semiconductor, the energy bands of which align with the CO/CO₂ and H₂O/O₂ potentials. Herein we report the synthesis of a unique p-n-p heterojunction material architecture, Cu₂O/S-doped TiO₂ micro-blocks covered with CuO nanowires, using anodization and annealing processes. The photocatalytic material shows excellent performance in the photocatalytic conversion of CO₂ and water vapor to methane under AM 1.5G illumination. The heterojunction material architecture exhibits a methane yield of 2.31 $\mu\text{mol m}^{-2} \text{h}^{-1}$, a rate approximately ten times higher than TiO₂ nanotube array films synthesized using similar anodization conditions. The improved performance of the heterojunctioned material architecture appears due to improved light absorption and efficient separation of the photogenerated charge.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ENVR.O-4

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 09:45, Chair: Dongwook Kim

High coke resistance for dry reforming of methane reaction over Ni/BaZrO₃ catalysts by temperature regulated chemical vapor deposition

Soong Yeon Kim, Uhm Sunghyun^{1,*}

Environment & Energy Research Team, Institute for Advanced Engineering, Korea

¹*Institute for Advanced Engineering, Korea*

Dry reforming of methane has potential benefits from the environmental perspective as it involves the destruction of two greenhouse gases that can be produce the syngas. $\text{CH}_4 + \text{CO}_2 \rightarrow 2 \text{CO} + 2 \text{H}_2$ $\Delta H^\circ = 247 \text{ kJ/mol}$ Dry reforming of methane reaction has studies with transition metals and noble metals. Noble metals are show higher activity and stability than transition metals towards dry reforming of methane reaction, however noble metal is limited to industrial application by high cost. The nickel catalyst has attracted its high activity and low cost compared with noble metal catalyst, but is weak for coke deposition which leads to catalytic deactivation. Therefore, it is necessary to study the catalyst with resistance to coking. In the previous study about nickel based catalysts, the coke deposition is effected on the kinds of support materials. In general, metal support catalysts are prepared by wet impregnation of various support. This method is not uniform in the metal dispersibility of the surface and requires a multi-step process, which makes it difficult to industrial application. Therefore, we proposed new concept of the catalytic preparation which is temperature regulated chemical vapor deposition that is simple process than wet impregnation and is a method of sublimation of the solid precursor to dry coating the support. In this study, to reduce coke deposition, the perovskite such as BaZrO₃ is used to support materials. The perovskite supported nickel catalyst is evaluated catalytic activity and coke resistance in dry reforming of methane reaction.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.O-5

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 10:10, Chair: Dongwook Kim

Electrochemical CO₂ conversion in aqueous solution via Copper Cluster

Yong-Jin Lee, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Many efforts are underway to convert carbon dioxide, a major contributor to global warming, into useful chemicals. Among them, conversion of carbon dioxide by an electrochemical method is known as a promising method, but since carbon dioxide itself is very stable and relatively inert, a lot of energy input is required for the CO₂ conversion. We have recently found that the application of Cu₃₂ clusters, whose structure is well defined, as an electrochemical catalyst, can convert the carbon dioxide in aqueous solution from low potential to formic acid. Previous computational chemistry studies have shown that the presence of hydride in the lattice structure of Cu₃₂ can provide the proton necessary for the conversion of carbon dioxide, especially in the form of formic acid production in competition with carbon monoxide and hydrogen. Therefore, Cu₃₂ clusters were used as a catalyst for the electrochemical conversion of carbon dioxide. In this study, carbon paper casted with Cu₃₂ was used as a working electrode and the formation of carbon monoxide, hydrogen and formic acid were detected by gas chromatography and NMR. As a result, the Cu₃₂ Cluster produces HCOOH (as HCOO⁻ at pH 6.8) at low overpotentials (89% at 0.3 V and 83% at 0.4 V), with minor amounts of CO and H₂. Thus, the present experimental results can provide a mechanism for the unique selectivity of the transition metal-based carbon dioxide conversion process having a hydride form.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ENVR.O-6

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 10:25, Chair: Dongwook Kim

Adsorbents based on Cross-linked Cyclodextrin Hydrogels for Removal of Organic Contaminants in Water

Ji Hwan Lee, Seung-Yeop Kwak*

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

Organic contaminants such as phenolic compounds and chlorinated compounds become serious problem threatening human health and ecosystem integrity. Simple and effective methods are presented here to prepare adsorbents by cross-linking cyclodextrin with diglycidyl ether and branched polyethyleneimine for the removal of organic contaminants in water. The cross-linked cyclodextrin hydrogels are capable of adsorbing organic contaminants by forming the inclusion complex. The properties of cross-linked cyclodextrin were characterized via FT-IR, N₂ adsorption-desorption analysis, FE-SEM. The adsorption properties of cross-linked cyclodextrin for bisphenol A as a model compound were measured by UV-vis. spectroscopy. Therefore, these results suggest that the cross-linked cyclodextrin has a great potential for efficient adsorbent for the removal of organic contaminants in water.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.O-7

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 10:40, Chair: Dongwook Kim

Development of Dynamic Multi-functional Membrane by Thermo-reversible Assembly of Heavy-metal Responsive Materials

Seung-Hwan Byun, Seung-Yeop Kwak*

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

In this study, we synthesize the phthalocyanine derivatives and Hyperbranched Poly (amidoamine) (HPAMAM) with maleimide groups and prepared the furan modified PTFE membrane. The maleimide modified Pc and the maleimide modified HPAMAM are reacted to the furan modified PTFE membrane by Diels-Alder (DA) reaction, resulting in the HPAMAM/Pc-modified membrane capable of optically detecting and capturing the chromium ion. When the chromium containing aqueous solution is permeated to HPAMAM/Pc-modified membrane, the fluorescence emission peak at 400 nm and 600 nm attribute to the Pc moiety at the membrane surface is significantly decreased due to the electron-quenching, indicating complex formation between Pc at the membrane surface and chromium ion. Furthermore, heavy-metal adsorption performance and water permeability of the membrane was improved via hydrophilic property of HPAMAM layer. In addition, the HPAMAM and Pc moiety saturated by chromium could be removed from the membrane and the new unsaturated HPAMAM, Pc moiety is functionalized again at the membrane surface through peel-and-stick method based on the DA and retro DA (rDA) reaction. This shows the successful development of the regenerable membrane that can simultaneously detect and remove heavy metal ions during the membrane water purification.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.O-8

Area: Current Trends in Environmental and Energy Chemistry

Type: Oral Presentation, Time: THU 10:55, Chair: Dongwook Kim

Removal of Tetrabromobisphenol A in Wastewater using a Sequential System of Bimetallic Nanoparticles and Enzyme

YOON-SEOK CHANG

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

Tetrabromobisphenol, TBBPA, is an efficient, reliable, and effective flame retardant, but concerns have been raised due to TBBPA's ability to leach into the environment and produce adverse effects on human health and ecosystems overall. This study investigated the degradation of TBBPA using an integrated system consisting of palladized zerovalent iron nanoparticles (Pd/nFe) and an oxidative enzyme, laccase. The Pd/nFe reductively debrominated TBBPA (> 90% of TBBPA) to produce bromo-free byproducts, including bisphenol A (BPA). After that, the metabolites, especially BPA, was rapidly oxidized by laccase in the presence of mediators. The influence of humic acid to activities of Pd/nFe and laccase in nano-enzyme hybrid system was also investigated. The effect of humic acid on remediation efficiency was not significant. In our study, we also observed that NPs treatment and wastewater components are factors which can reduce activity of laccase in BPA degradation. As a result, laccase was encapsulated in the copper-alginate beads (lac-bead) to maintain its activity. The lac-bead system was able to remove over 90% of BPA after 24 h in both NPs treated and wastewater solutions. The results indicate that the nano-enzyme remediation system is a simple remedying system with high pollutant removal efficiency in complex contaminated sites.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-1**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Iron-Catalyzed Direct Azidation of Polybutadiene and Consecutive Click-Reaction

Haeji Jung, Yeong Gweon Lim^{*}

Agency for Defense Development, Korea

Azides have been widely utilized as precursors leading to formation of amines and synthesis of nitrene. Therefore organic azides have played important role in various scientific fields. Numerous synthetic protocols and applications have been developed, but there are a few reports describing the direct azidation of polymer. Recently, several groups obtained azido-functionalized polymer by using combination of trimethylsilyl azide and iodine compound through single-step substitution reaction. In this work, the research on synthesis of azidated phenyl-terminated polybutadiene(PtPB) introduced azide groups to alkenes was described. Polybutadiene is appropriate for prepolymer applied to binder of composite propellants due to their excellent mechanical properties, sufficient desensitization toward impact and friction, and good low-temperature elongation. To improve the weakness of polybutadiene such as non-energetic polymer, introduction of azide groups into PB was conducted. Synthesis of three different types of azidated PtPB having 5, 10, 15% substitution rates was established by iron-catalyzed radical reaction under optimized reaction conditions. Moreover, resulting azido-functionalized PtPBs were reacted with alkyne to obtain the triazole-containing polymer.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-2**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

One-Pot Synthesis of Hyperbranched Polyamines Based on Novel Amino Glycidyl Ether

Songa Kweon, Gyunhyeok Ahn, Byeong-Su Kim*

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

We report a one-pot synthesis of hyperbranched polyglycerols possessing amino functionality by using a novel Boc-protected aminoethanol glycidyl ether monomer (BAG). A series of hyperbranched Boc-protected polyamino glycerols (PBAG) were prepared through a one-pot anionic ring opening multibranching polymerization to yield PBAG with controlled molecular weights (3500–17400 g/mol) and relatively low molecular weight distributions (1.2–1.8). Subsequent deprotection of PBAG yielded hyperbranched polyamino glycerols (PAG) with a globular polymeric structure that comprises a randomly branched structure with a large number of amine and hydroxyl groups. ¹H, ¹³C, and ¹⁵N NMR, GPC and MALDI-TOF measurements confirmed the successful polymerization of the hyperbranched PAG polymers. With its superior biocompatibility of PAG, we anticipate the prospective potentials for the applications in biological and biomedical fields.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: POLY.P-3

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Highly Efficient Regioregular Terpolymers Containing Fluorine Atoms on Bithiophene Segment Processed from Halogen-Free Solvent

Soyoung Jang, YOUNGU LEE*

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

Organic solar cells (OSCs) have attracted significant interest due to cost-effective, lightweight, flexibility and large-area fabrication. Bulk heterojunction (BHJ) in which typically a donor polymer is blended with electron acceptor material such as fullerene derivative has been predominantly used as a typical active layer. However, in order to overcome the limitations of the alternating push-pull chain approach, terpolymer design with regioregular alternating D1-A-D2-A strategy has been explored intensively for designing efficient electron donor. Recently, we synthesized a new series of fluorinated benzothiadiazole (FBT)-based terpolymers comprising two donating units, quaterthiophene (QT, D1) and benzo[1,2-b:4,5-b']dithiophene (BDT, D2). Furthermore, we introduced two and/or four fluorine atoms on bithiophene unit and called them PfBT4T-BDT, PfBT4T2F-BDT and PfBT4T4F-BDT, respectively to investigate how increasing the number of fluorine atoms affects the physical properties and OSC device performances. Due to fluorine substitution, PfBT4T2F-BDT and PfBT4T4F-BDT showed deeper HOMO level compared to PfBT4T-BDT. In addition, increase of the number of fluorine atoms from 0 to 4 led to enhanced absorption coefficients and promoted exciton dissociations due to suppressed recombination process, thus remarkably improved Jsc values. Therefore, the bulk-heterojunction OSC device based on PfBT4T4F-BDT and diphenylether (DPE) additive showed a high power conversion efficiency (PCE) of 8.45%, while the OSC devices based on PfBT4T-BDT, PfBT4T2F-BDT with DPE exhibited PCE of 6.15% and 7.54%, respectively.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-4**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Room-Temperature Synthesis of Widely Tunable Formamidinium Lead Halide Perovskite Nanocrystals: A New Candidate for Optoelectronic Devices

DUONG NGUYEN MINH, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

Colloidal perovskites nanocrystals based on formamidinium lead halide (FAPbX₃) have been synthesized by ligand assisted reprecipitation method using PbX₂-DMSO complexes as precursors at room temperature. Well-defined cubic-shaped FAPbX₃ nanocrystals have been obtained with a size of $d = \sim 10$ nm. The synthesized FAPbX₃ nanocrystals show bright photoluminescence with a high photoluminescence quantum yield (PLQY for FAPbBr₃ = 75%). The lifetimes of FAPbBr₃ nanocrystals were measured for the samples isolated at several different centrifugal speeds. The photoluminescence is able to be tuned from blue to near infrared region ($\lambda_{\text{peak}} = 408\text{--}784$ nm) either by changing the amount of oleylamine or the composition of X. The color expression range is 135% of NTSC standard. The band width of the photoluminescence spectra of FAPbX₃ nanocrystals is narrow (FWHM = 18–48 nm). FAPbX₃ nanocrystals show better thermal stability than MAPbBr₃ nanocrystals.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-5**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Eutectic melting process for guiding single crystallization : The Effect on the molecular structure of Poly(9,9-di-n-octylfluorene-alt-benzothiadiazole) by eutectic melting and annealing

Sangheon Lee, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

Highly ordered polymer packing is important for organic electronic device because of intra- and interchain charge transport. It is well known that annealing process above glass transition temperature makes polymer be more stable state and have high ordered structure. Many people use thermal annealing process after spin-coating their semiconducting polymer. We found that crystallizable additives such as naphthalene and 1,3,5-trichlorobenzene give highly ordered structure to Poly(9,9-di-n-octylfluorene-alt-benzothiadiazole), which is called 'F8BT'. Through Eutectic melting, additives and F8BT can be mixed homogeneously. By cooling mixture, additives are crystallized and it helps F8BT to have ordered structure. Interestingly, when our film with using eutectic melting was annealed at same condition with pristine film, it has more complicated and higher ordered structure. The films were analyzed by grazing incidence wide angle of x-ray Scattering(GIWAXS), AFM, and FT-IR. It was confirmed that GIWAXS of annealed structure with eutectic melting has many diffraction peaks at face-on, which means lamellar supramolecular structure.

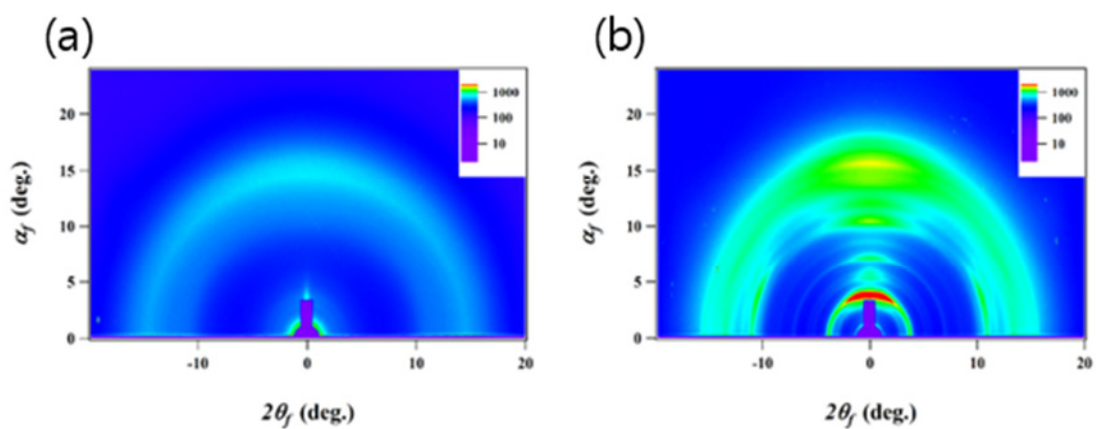


Figure 1. 2D GIWAXS patterns of the F8BT film of pristine (annealed at 150 °C) (a) and eutectic melted with Naphthalene (annealed at 150 °C) (b)



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-6**

Area: Polymer Chemistry

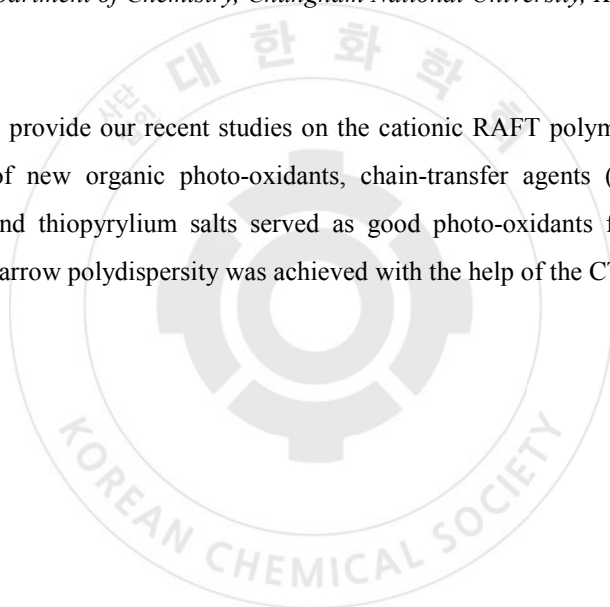
Type: Poster Presentation, Time: FRI 13:00~14:30

Photocontrolled Cationic RAFT Polymerization of Vinyl Ethers

Soo won Jang, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

In this presentation, we provide our recent studies on the cationic RAFT polymerization of vinyl ethers using a combination of new organic photo-oxidants, chain-transfer agents (CTA), and visible-light irradiation. Pyrylium and thiopyrylium salts served as good photo-oxidants for initiating vinyl ether polymerization, while narrow polydispersity was achieved with the help of the CTAs.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-7**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of quaternized ammonium salt acrylate polymer from 2-dimethylamino ethyl methacrylate and dimethyl sulfate as an antibacterial polymer

JI EUN JO^{*}, Chang Woo Han¹, Kyungtae Park¹

Research and Development, KD Chem Co., Korea

¹*Research and Development, KD Chem CO., Korea*

In general, the antibacterial agent applied to the antibacterial filter for air cleaners is mainly composed of a low-molecular type substances. As time elapses, the antimicrobial effect deteriorates due to the desorption, and the desorbed substances spreads into the air, which has a bad influence on health. To solve this problem, a quaternary ammonium salt acrylic polymer was applied to an antibacterial filter. Acrylic polymers with fixed strength are slow to release and thus have a continuous antibacterial effect. It is well known that quaternary ammonium salts are cationic and have an antibacterial effect. First, to synthesize the quaternary ammonium salt was used DMAEMA (2-Dimethylaminoethylmetacrylate) as the tertiary amine and DMS (Dimethylsulfate) as the cationic agent. The reaction between DMAEMA and DMS was exothermic and showed the highest yield of 96.5% at reaction ratio (DMS / DMAEMA) of 1.2 and reaction temperature of 45 °C. Quaternary ammonium salt acrylic polymers were synthesized by emulsion polymerization using DMAEMA-DMS of 18.0% , Ethyl acrylate of 11.0% , Glycidyl methacrylate of 4.0% , Acrylic acid of 2.0%, Methyl methacrylate of 2.5%. The synthetic quaternary ammonium acrylate polymer showed 99.9% antibacterial activity against Staphylococcus aureus and Pneumococcus by the shaking flask method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-8**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Bioinspired Catecholic Primers for Rigid and Ductile Dental Resin Composites

Eeseul Shin, Sung Won Ju¹, Larry An¹, Jin Soo Ahn^{1,*}, Kollbe Ahn^{1,*}, Byeong-Su Kim^{*}

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

¹*Marine Science Institute, University of California, Korea*

In the construction of dental restorative polymer composite materials, surface priming on mineral fillers is essential to improve the mechanical performance of the composites. Here we present bioinspired catechol-functionalized primers (catechol-spacer-methacrylate) for a tougher dental resin composite containing glass fillers. Catecholic primers with different end groups were designed and then coated on glass surfaces using a simple drop-casting or dip-coating process. The surface binding ability and possible crosslinking (coupling or chemical bridging between the glass substrate and the dental resin) of the catecholic bifunctional primers were evaluated using atomic force microscopy, contact angle measurements, and the knife shear bonding test and compared to a state-of-the-art silane-based coupling agent. Various mechanical tests including shrinkage and compression tests of the dental resin composites were also conducted. Compression tests of the composites containing the catecholic primed fillers exhibited enhanced mechanical properties, owing to the bidentate hydrogen bonding of catechol moieties to the oxide mineral surface. Furthermore, the superior biocompatibility of the primed surface was confirmed via cell attachment assay, thus providing applicability of catecholic primers for practical dental and biomedical applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-9**

Area: Polymer Chemistry

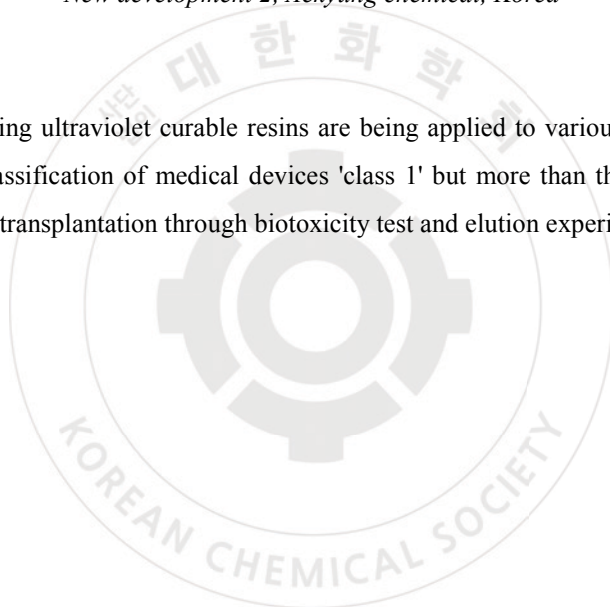
Type: Poster Presentation, Time: FRI 13:00~14:30

3D PRINTING INKS FOR DENTAL MATERIALS APPLICATION

Sangwon Park, YOON TAE JEON*

New development 2, Aekyung chemical, Korea

Inks for 3D printing using ultraviolet curable resins are being applied to various medical fields. We are developing not only classification of medical devices 'class 1' but more than the 'class 2' ink. We have tested the possibility of transplantation through biotoxicity test and elution experiment.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-10**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Controlled Synthesis of Sodium Polystyrenesulfonate via Atom Transfer Radical Polymerization and Coupling of Polystyrene Beads Selectively at the Terminal Units

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Synthesis of anionic polyelectrolyte sodium polystyrenesulfonate (NaPSS) with predetermined molecular weight, low polydispersity index (PDI), and controlled kinetics has been carried out. The monomer styrene with a sulfonate group at its para-position has been homopolymerized in water/methanol (1:1, volumetric) mixed solvent media, which controlled the rate of polymerization. Initially, the molecular weight of the polyelectrolyte was determined by ¹H-NMR spectroscopy. To reconfirm, it was also determined using Gel Permeation Chromatography (GPC) technique and the PDI was evaluated to be about 1.2. Characterization of the polymer was carried out using ¹H-NMR, ¹³C-NMR, and FT-IR. One of the two terminal groups contained –COOH group introduced into the chain through the initiator while the other end was having the –Br group which came via atom transfer from the copper catalyst complex. A polystyrene bead (diameter 2 μm) with –NH₂ groups on its surface was linked to the terminal unit containing –COOH group through amide bond formation. Thereafter, the –Br group at the other terminal unit was converted to –COOH group which was then coupled to another polystyrene bead bearing –NH₂ group. This strategy of successive addition of polystyrene beads to the polyelectrolyte chain helped us to negate the possibility of linking of both the ends of a chain into the same bead resulting controlled coupling of two beads per polymer chain. These beads-linked polyelectrolyte chains will be used to study their coiling/uncoiling behavior via single molecule spectroscopic technique, such as, optical tweezer.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-11**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Miscible Epoxy-based Perfluorinated Additives for Anti-fingerprint Properties of Flexible Hard Coating and Development of Film Preparation Protocols

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In flexible displays, both hardness and flexibility are required to give durability during bending or folding of the screen. To satisfy these requirements, hybrid organic-inorganic materials are widely used. Especially, a silica-based hybrid hard coating film is known to exhibit high pencil hardness, flexibility, and outstanding transparency. However, after curing the hard coating film, it is difficult to introduce another coating layers on the cured film due to the lack of functional groups to react on the surface. One of the strategies to introduce anti-fingerprint (AF) property on the hard coating surface is to add a little amount of curable perfluorinated materials to the film forming solution. This approach is attractive because only a small amount of expensive fluorine-based materials is used, maintaining the hardness of hard coating itself. For example, Daikin Industries, Ltd. was developed an AF additive for hard coating, OPTOOL™-DAC HP. However, this cannot be utilized in epoxy-based hard coating materials because it has acrylate as a curable group. In this research, we have synthesized an epoxy-based AF additive with a long poly(perfluoropropylene oxide) chain for hard coating and developed a film preparation protocol in which less than 1 wt% of the synthesized additive is employed. From inexpensive tris(hydroxymethyl) aminoethane, we introduced three epoxy groups in one molecule as a dendritic structure for high degree of curing reaction and high miscibility with hard coating components. We then optimized the film preparation protocol to obtain hard coating film exhibiting AF properties with the lowest amount of the additive. The prepared AF films showed high water and ink repellency without any loss of inherent hardness of hard coating.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-12**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fabrication nanoporous structure of M13 virus/PolyDADMAC

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Recently, studies using biocompatible materials have received much attention regardless of field. In addition, studies using a self-assembly technique capable of relatively simple fabrication of a precise shape and a nanostructure have been actively conducted. In this study, various self-assembly structures based on the M13 virus, a biocompatible biomaterial with a very constant structure and morphology, were constructed. And the M13 virus can express various characteristics through genetic engineering methods, so it is highly applied and utilized. We fabricated nano-porous laminated structure of M13 virus by self-assembly technique. We have confirmed through the fabrication model that at initial rough surface layers condition followed up by porous surface on top, as number of alternative layers were deposited. The structure of final layer is composed of pore diameter ~150nm – 500nm (± 20 nm) and height of ~15nm – 30nm (± 5 nm). We expect to be able to obtain interesting results in areas such as ion filter, SPR and sensors etc.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-13**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Single-Electron Transfer Living Radical Polymerization and Reactivity Ratios of Functionalized Methacrylate Monomers

Jongwon Choe, SOO HYUN LEE¹, Keewook Paeng¹, Myungwoong Kim^{*}

Department of Chemistry, Inha University, Korea

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Controlled radical polymerization (CRP) is one of utilized tools for polymer synthesis due to its ability to achieve low dispersity, tailored functionality, and complex structure simultaneously. Among the CRP methods, single-electron transfer living radical polymerization (SET-LRP) has attracted attentions as molecular weight can be easily controlled at both low and high molecular weight regimes while preserving target functionalities. Herein, we demonstrate random copolymerization of functionalized methacrylate monomers by Cu(0)-mediated SET-LRP and calculate reactivity ratios of each monomer against methyl methacrylate by ¹H NMR spectroscopy. Relatively similar composition of resulting copolymers is obtained compared to feed ratio of monomers. Density of functionalized site of copolymers can be easily controlled and expected by initial composition.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-14**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Simple Method to Fabricate a Janus Membrane via Post-Electrospinning Functionalization of Reactive Random Copolymers

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Department of Chemistry, Inha University, Korea

We demonstrate the fabrication of a Janus membrane, exhibiting different physical/chemical properties of one side from the other, by post-electrospinning functionalization of electrospun polymeric nanofibers. The nanofiber consisted of poly(styrene-*random*-glycidyl methacrylate), namely P(S-*r*-GMA), where dopamine is incorporated in only one side *via* post-electrospinning modification. Since epoxy groups in GMA can react with strong nucleophiles such as amine, hydroxyl, and thiol groups; the electrospun P(S-*r*-GMA) nanofibrous mat was functionalized with amine in dopamine by floating on the surface of an aqueous reactant solution and subsequent heating. Incorporation of dopamine was confirmed by Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy, and contact angle measurements. Resulting membrane was further utilized for catching metallic particles using the metal adhesion characteristic of catechol group. Our results will provide an effective route to facilitate the fabrication of Janus membrane using electrospinning of reactive polymers.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-15**

Area: Polymer Chemistry

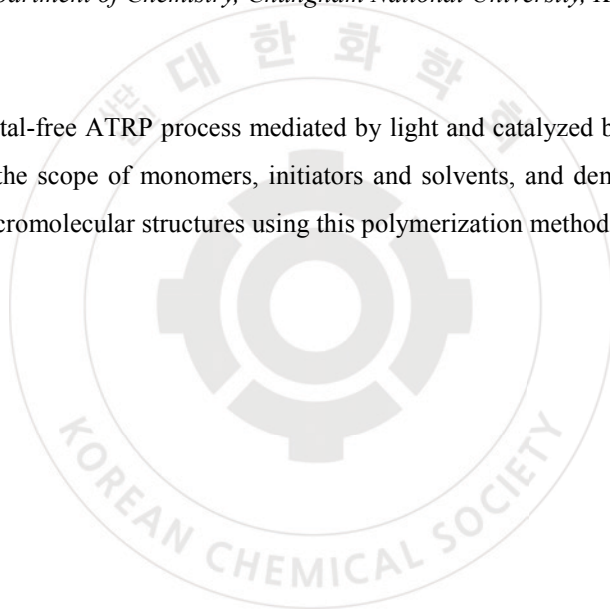
Type: Poster Presentation, Time: FRI 13:00~14:30

Photoinduced Metal-Free Atom Transfer Radical Polymerization

Gyeong Su Park, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

We investigated the metal-free ATRP process mediated by light and catalyzed by an organic photoredox catalyst. We extended the scope of monomers, initiators and solvents, and demonstrated the successful synthesis of diverse macromolecular structures using this polymerization method.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-16**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Synthesis of Degradable Poly (styrene-block-ethylene glycol) via Staudinger Reaction

Suhong Park, Sol An, Haebin Kim¹, Sang Sik Woo, Myungwoong Kim, Dong Wook Kim^{*}

Department of Chemistry, Inha University, Korea

¹*Inha University, Korea*

The Staudinger reaction employing azide and phosphine is rapid in the presence of water and has high chemoselectivity. Through Staudinger reaction, block copolymers possessing triarylphosphine as a junction point enable to decompose or change one part of block copolymers. We have synthesized degradable block copolymers using styrene, methoxy ethylene glycol(mPEG), and triarylphosphine. The block copolymers were characterized by ¹H NMR and gel permeation chromatography(GPC). The mPEG part in resultant block copolymers was removed by organic azide compounds through Staudinger reaction. The synthesized block copolymer is anticipated introducing other functionalized molecules.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-17**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Characterization of Poly(amide-imide)s Containing Fastened Alicyclic Rings

Seong jong Kim, Sang Youl Kim *

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

Among the high temperature polymers, poly(amide-imide)s have been investigating as one of promising materials due to high thermal stability and mechanical properties with balanced processability. Also, several properties such as thermal stability, optical property and thermo-dimensional stability could be regulated by modifying monomer structures. In this study, we synthesized two diacid monomers, one containing a alicyclic ring, which is fastened with phenyl pendant groups, and the other containing biphenyl with bulky trifluoromethyl groups symmetrically. Using these synthesized diacids and 2,2'-bis(trifluoromethyl)benzidine, PAIs were prepared by polyamidation and converted to a film by solution casting in DMAc. It's detail synthetic route and properties will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-18**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Monodisperse Hyperbranched Polymer Nanoparticles: Surfactant-free Synthesis, Characterization and Functionalization

Yesin Lee, Byeong-Kwan An*

Department of Chemistry, The Catholic University of Korea, Korea

Monodisperse polymer nanoparticles with reactive functional groups on the surface have contributed significantly to progress in a variety of fields of chemical, mechanical, biomedical, environmental and photoelectric applications. In this study, we prepared the monodisperse hyperbranched polyester nanoparticles which contain surface phenolic groups by one-pot surfactant-free polymerization. The size, shape and surface properties of the obtained polymer nanoparticles were characterized by dynamic light scattering (DLS), FE-SEM, zeta potential and pH measurements. The functionalization of surface phenolic groups of the polymer nanoparticles was carried out by reaction with carboxylic acid-containing fluorescent dye molecules.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-19**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of pH-responsive Diblock Copolymer poly(4-hydroxystyrene-*b*-*N*-vinylamine) by using RAFT polymerization

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Poly(*N*-vinylamine) (PVAm) an interesting polymer which is the simplest amine containing polymer. However, synthesis of PVAm is challenging problem, the monomer can undergoes tautomeric imine and forming undesired complex condensation. So, there have been few reports about synthesis of PVAm through controlled radical polymerization. We synthesized poly(4-hydroxystyrene-*b*-*N*-vinylamine) (PHS-*b*-PVAm) by using Reversible Addition Fragmentation Chain-Transfer (RAFT) polymerization. We use 'switchable' RAFT agent to make poly(*p*-acetoxystyrene-*b*-*N*-vinylformamide) (PACOS-*b*-PNVF), the precursor of PHS-*b*-PVAm, in which reactivity of the active C-S double bond on thiocarbonyl group, by protonation/deprotonation of Z group of RAFT agent. This agent gives unusual, good control over the polymerization of both PACOS and PNVF block. Hydrolysis of PACOS-*b*-PNVF gives diblock polyampholyte PHS-*b*-PVAm which has acidic phenolic moiety on hydroxystyrene block and basic primary amine on vinylamine block. The resulting polymer self-assembled in water, forming spherical micelle nanoparticles. Also, it shows pH-responsive character for both acidic and basic condition.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-20**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Photocatalytic Thiol-Ene Click Reaction Using Visible Light for Postpolymerization Modification

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Thiol-ene click reaction is highly efficient and rapid reaction to achieve quantitative yield with no side reaction. The reaction can be triggered by photoredox catalysis in the presence of dye molecules. Among a variety of dye molecules, Eosin Y has attracted attentions as a photoredox catalyst because it is metal-free and hence, environment friendly, commercially available with low cost, efficient in photocatalysis due to its high quantum yield at visible light wavelength range. We demonstrate the photocatalysis with visible light illumination to modify reactive copolymers having various alkene groups which can be functionalized with thiol containing molecules. The postpolymerization modifications in this study emphasize the potential of visible light-mediated thiol-ene click chemistry to accomplish target structures in polymeric materials towards desired physical and chemical properties.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-21**

Area: Polymer Chemistry

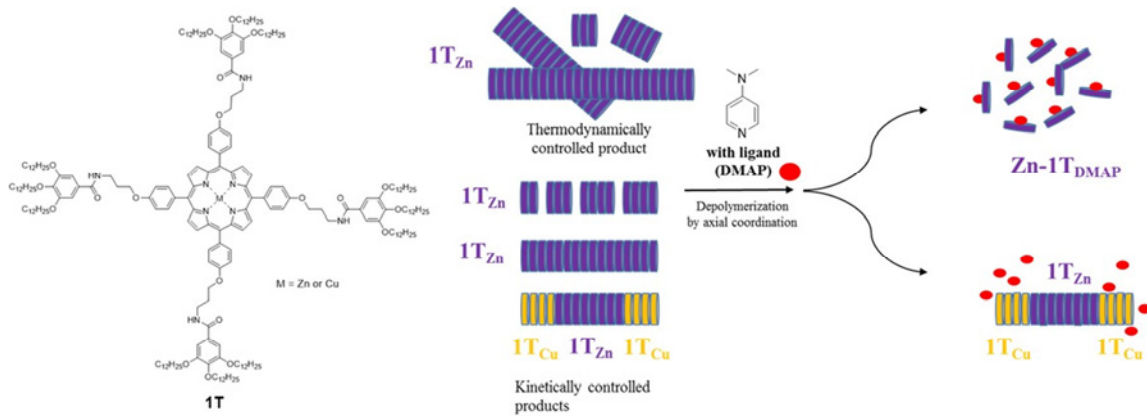
Type: Poster Presentation, Time: FRI 13:00~14:30

Probing kinetic stability of supramolecular polymers in terms of their composition

Sung Ho Jung, Kazunori Sugiyasu^{*}, Masayuki Takeuchi^{*}

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Kinetic insight into supramolecular polymerization allows for the control over self-assembled nanostructures. For example, we have recently achieved living supramolecular polymerization, which enabled us to synthesize supramolecular polymers with controlled length and narrow polydispersity.[1,2] This method is expected to lead to the synthesis of supramolecular block copolymers, yet doing so remains a great challenge. Herein, supramolecular copolymerization of two different porphyrin derivatives complexed with either zinc or copper ($1T_{Zn}$ or $1T_{Cu}$, respectively) as metal core was investigated. These two different porphyrins can coassemble because of their structural similarity. Through the seeded-growth approach, which we have previously established[1,2], we succeeded in the extension of the block of $1T_{Cu}$ stack from the $1T_{Zn}$ seed, thereby creating the supramolecular block copolymer ($1T_{Cu}-1T_{Zn}-1T_{Cu}$). Interestingly, the end-capped supramolecular block copolymer ($1T_{Cu}-1T_{Zn}-1T_{Cu}$) showed the enhanced kinetic stability in comparison with non-protected supramolecular polymer at terminal part ($1T_{Zn}-1T_{Zn}-1T_{Zn}$) against axial ligand (DMAP). We believe that this approach will expand the understanding on kinetic insight and potential application of supramolecular polymerization.[1] S. Ogi, K. Sugiyasu, S. Manna, S. Samitsu, M. Takeuchi, Nat. Chem., 2014, 6, 188-195.[2] T. Fukui, S. Kawai, S. Fujinuma, Y. Matsushita, T. Yasuda, T. Sakurai, S. Seki, M. Takeuchi, K. Sugiyasu, Nat. Chem., 2017, 9, 493-499.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-22**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Permeation-induced chromatic change of polydiacetylene vesicle

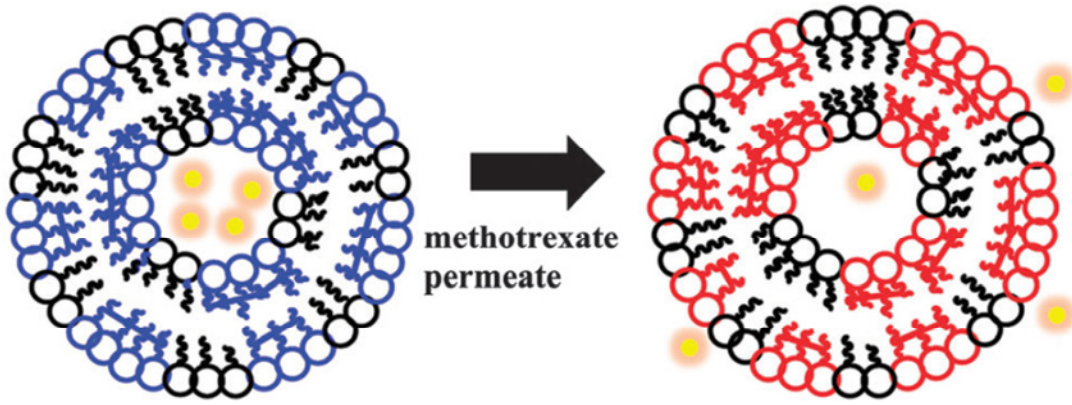
Min Jae Shin, Young Jae Shin^{1,*}, Jae Sup Shin^{2,*}

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²Department of Chemistry, Chungbuk National University, Korea

The noble vesicular system of polydiacetylene showed a red shift by two kinds of detecting systems. One of the systems involves absorption of target materials from outer side of the vesicle, and the other system involves the permeation through the vesicular layers from within the vesicle. The chromatic mixed vesicles of N-(2-aminoethyl)pentacosyl-10,12-diamide were formed with dimethyldioctadecylammonium chloride or tetra(ethylene glycol) monoctadecyl ether by sonication, followed by polymerization by UV irradiation. Methotrexate was used as a target material. The polymerized mixed vesicles showed the blue color, and a red shift was observed indicating the adsorption of methotrexate on the polydiacetylene bilayer. In order to check the chromatic change by the permeation of methotrexate, we separated the vesicle portion, which contained methotrexate inside the vesicle, and checked chromatic change during the permeation of methotrexate through the vesicle. The red shift apparently indicates the disturbance in the bilayer induced by the permeation of methotrexate. The molar ratios in the mixed vesicles which showed the maximum contrast of color were determined. The change color could occur through permeation of a substrate with a high molecular weight, for example gentamicin and neomycin, but it could not occur with a substrate with low molecular weight, for example ethylamine and butylamine.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-23**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Chromatic detection of glucose by polydiacetylene vesicle

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Research on the glucose sensor is particularly very noteworthy, because of increasing diabetics around the globe. People with diabetes must measure their sugar levels in their blood several times a day. Recently, many new methods for detecting glucose have been reported. Polydiacetylene (PDA) vesicle is formed by the sonication of an amphiphilic diacetylene compound, following UV irradiation. The color of the PDA vesicle is changed from colorless to blue during polymerization. Glucose oxidase is known to react with glucose to promote the oxidation reaction as follows. $\text{Glucose} + \text{O}_2 \rightarrow \text{Gluconic acid} + \text{H}_2\text{O}_2$. And H_2O_2 can be used as an initiator for the polymerization of a diacetylene compound, and the polymerization process was used for sensing, i.e., the transition from a colorless monomeric vesicle state to a polymerized blue state was used as a sensing step for H_2O_2 . Therefore, in this study a polydiacetylene vesicle was used to fabricate glucose sensor, allowing feasible colorimetric detection. The vesicle was formed by sonication of 10,12-pentacosadiynoic acid (PCDA). H_2O_2 formed by the reaction between glucose and glucose oxidase functioned as the initiator for the polymerization of PCDA in the presence of horseradish peroxidase. The solution turned blue after the polymerization of PCDA vesicle. Thus the glucose concentration could be detected to the concentration level that turns the solution to blue. The UV absorbance of glucose solution was proportional to glucose concentration. The results of this study indicate that glucose concentration upto 1 mM can be detected by change in blue color by eyes. We believe that a sensor capable of colorimetric detection of glucose concentration directly by eye will be meaningful.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-24**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Photovoltaic properties of conjugated low bandgap polymers having aromatic heterocyclic compounds(thiophene and selenophene) : a comparative study

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In this study, we investigated the photovoltaic properties of newly synthesized low bandgap conjugated polymers, P1-TCP (thiophene-based conjugated polymer) and P2-SCP (selenophene-based conjugated polymer). These two conjugated low bandgap polymers were characterized by NMR and gel permeation chromatography. The physical properties of the polymers were studied by thermogravimetric analysis. Moreover, we also investigated the optical, electrochemical and morphological properties of both polymers by UV-vis spectroscopy, cyclic voltammetry and atomic-force microscopy (AFM), respectively. Later, we studied the photovoltaic properties of both low bandgap polymers blended with PC61₆₁BM in different ratios with different thicknesses. In addition, post thermal annealing at different temperatures for both polymers was investigated, and the results show that P2-SCP exhibited stronger molecular orientation properties as compared to P1-TCP.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-25**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study of Supramolecular Polymerization of pH-dependent Hydrazone Pyridinium Conjugates

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Hydrazones, one of the most well-known functional group in the field of dynamic covalent chemistry, have been utilized to construct stimuli-responsive self-assemblies. However, the role of hydrazone was mostly a simple H-bonding donor, a molecular linker or a site for metal binding. In this study, we have designed and synthesized novel benzoyl hydrazone para-pyridinium conjugates which showed wire-type supramolecular polymers. The hydrazone dye molecules were pH-dependent that they disassembled in a basic solution. UV-vis spectroscopic data of mono-hydrazones (H1, H(Me), Hm) were collected to study the behavior of the dyes. The combination of an acid dissociation model and a dimerization model allowed us to examine the UV-vis spectra of H1, calculate each fraction of the dimer (D), hydrazone (H), and zwitterionic hydrazone (Z) upon changing its concentration. Furthermore, we obtained the crystal network structure of H1 by X-ray crystallography. We could figure out the intermolecular interaction of the hydrazone dyes by Hirshfeld surface analysis; the packing of H1 into the crystal is mainly occurred by CH- π and π - π stacking interactions, along with van der Waals and dipole-dipole interactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-26**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Self-healable Norbornene-based Supramolecular Polymer Gels by Metal-Terpyridine Interaction

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¹*Sungkyunkwan University, Korea*

Self-healing is an interesting property for prolonging the lifetime of materials, but the self-healing behavior is rarely observed and a spontaneous healing capability is especially uncommon. The repair process usually requires additional energy such as heat, light and specific solvent at the damaged area. In this study, we investigated self-healing property of norbornene-based polymers using self-assembly by metal-terpyridine interaction without any stimulus. The polymers were easily synthesized by ring-opening metathesis polymerization (ROMP) using Grubb's 2nd generation catalyst. To control the self-healing property, polymers with different ratios of norbornene-terpyridine (NB-tpy) and norbornene-ethylhexyl (NB-eh) were prepared. The metallo gels were easily generated by simply mixing the polymer solution and metal ions together. When various kinds of metal ions (Fe^{2+} , Zn^{2+} , Co^{2+} , or Ni^{2+}) are added to the polymer solution, we observed that the larger the binding constant between terpyridine and metal ion, the less amount of metal ions was necessary to form gels. Furthermore, we confirmed that the cutted gel can be self-healed in a short time (about 10-15 min.) without any additives.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-27**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study on the diffraction efficiency of the photosensitive polymers using ionic liquid

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Recently, it is getting important to information storage devices. So, we have focused on the epoxy-based materials for the information storage devices. In order to synthesized the photosensitive azo-polymer and studied the surface relief-grating (SRG) fabrication and real time image recording using diode-pumped solid-state (DPSS) laser of 532 nm, and diffraction efficiency (DE) of polymer using low power DPSS laser at 633 nm. But, the DE of synthesized polymer is low even after 15 min exposure. Hence, to increase the efficiency and reduce the time of DE measurements for synthesized polymer, we have investigated the SRG and DE with combination of azo-polymer and ionic liquids (ILs). We have used various ILs such as imidazolium and ammonium family ILs. For the first time, we observed that DE has increased awfully for DEAP-azo-polymer mixture in 4 min as compared to azo-polymer (alone) and other polymer-IL mixtures. Therefore, DEAP IL can help in increasing the efficiency of DE measurements in less time.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-28**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Interaction Studies between Newly Synthesized epoxy based azopolymer and Ionic Liquids

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Department of Chemistry, Kwangwoon University, Korea

In this information age, different kinds of photosensitive materials have been used in the manufacture of information storage devices. But these photosensitive materials have the bane of low diffraction efficiency. In order to solve this problem, we have synthesized a novel photosensitive polymer from epoxy-based azopolymers (with three types of azochromophores). Furthermore, we have studied the interaction between this newly synthesized azopolymer and ionic liquids (ILs). For this purpose, we have used diethylammonium dihydrogen phosphate (DEAP), tributylammonium methyl sulfate (TBMS), triethylammonium 4 aminotoluene-3-sulfonic acid (TASA), and 1-methylimidazoliumchloride ([Mim]Cl) ILs. To investigate the molecular interaction between azopolymer and ILs, we have used the following spectroscopic methods of analysis: UV-visible spectroscopy, photoluminescence (PL) spectroscopy, Fourier transformed infrared spectroscopy (FT-IR), and confocal Raman spectroscopy. In this study, we have developed new photosensitive materials by combining polymer with ILs.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-29**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Prediction of glass transition temperature of co-polymers based on quantitative structure-property relationship

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The glass transition temperature(Tg) is temperature at which the amorphous phase of the polymer is switched between the rubbery state and glass state. Tg is one of the most important properties of polymers. Tg depends on the measurement conditions and is difficult to determine experimentally because the transition occurs over a relatively wide temperature range. Polymers change its state based on glass transition temperature. Therefore, the prediction of glass transition temperature for polymers can be used to design new polymer with appropriate properties. In this study, quantitative structure-property relationships (QSPRs) study were conducted to estimate the glass transition temperature of copolymer. The molecular descriptor used in predictive model were calculated from the chemical structure using the PreADMET program. Multilinear regression (MLR) and support vector machine (SVM) were used as the learning method and their models were verified by internal and external validation method. And the prediction range of chemicals is set in kNN-based applicability domain(AD) of the model.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-30**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

QSPR modeling for solubility parameter of polymers

KYUSUNG LEE, Byeong Hun Lee, Yong Seok Kim¹, Sung Kwang Lee*

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The solubility parameter is a characteristic of a liquid which is a measure of component mixing. The solubility parameter applies the principle of "like dissolve like". In other words, if the interactions between substances are similar, they are similar in properties to each other and can dissolve well, so this is the best way to compare the solubility parameters. The solubility parameter concept based on regular solution theory has been extensively used in practical applications of polymers in various solvents and solvent mixtures. It has proven to be a valuable empirical tool in the paint and lacquer industry and in the prediction of adhesive interactions. A polymer is composed of long chains of regular repeating units due to the chemical reaction of monomers. Polymer materials are used in variety of area such as aerospace, energy and IT industry. Several physicochemical properties are used to characterize these polymers. In this study, we have developed QSPR(quantitative structure-property relationship) models for predicting solubility parameter of polymer from 2D chemical structure. Multiple linear regression and support vector machines were used to learn the model using descriptors related to solubility parameters. And y-scrambling and cross validation were used to verify the stability and predictability of the model. Finally, applicability domain of models could be used to specify the scope of the models. These models show that they can be used to predict the solubility parameter of a wide range of polymers.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-31**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fabrication of porous PS/PMMA microspheres through pickering emulsion

Jeong rae Kim^{*}, Daewon Sohn^{*}

Department of Chemistry, Hanyang University, Korea

Porous polymer particles have attracted great interests due to numerous applications in many areas of advanced materials science. This research shows fabrication of porous SPS/PMMA(Sulfonated polystyrene/Poly methyl methacrylate) microspheres using γ -ray radiation and pickering emulsion. Porous SPS/PMMA microspheres has different pore sizes. The PS(Polystyrene) particles were located at interface between water and monomer. They can form pickering emulsions by shear force. Then, monomer will be absorbed into particles because of swelling properties of PS particles and water also diffuse into the particles by osmosis. These two factors induce the pores on the particles. They show different pore sizes and morphology depending on sulfonation time and swelling time. In this research, the porous microspheres are prepared via seeded polymerization with γ -ray radiation which didn't require any chemicals as initiator and crosslinker.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-32**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Heavy metal ions adsorption by synthesized HNT/EDTMP nanocomposite

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Halloysite/EDTMP, which is made of condensation reaction of alumina and phosphonic acid, has been newly synthesized. The P-O-Al linkage of halloysite surface is probable by covalent bond of alumina and phosphonic acid, which makes strong bidentate and tridentate bond. The remained phosphonic acid parts of EDTMP could easily bind to plus charged ions in the solution. This enables reaction of metal ions and reactive reagents, which is also known as chelating, would be helpful to collect heavy metal ions in solutions. The hybrids would be characterized by means of scanning electron microscopy and IR spectrometry. IR spectroscopy would be for proving bidentate or tridentate P-O-Al linkage of HNT/EDTMP, and chelating bonds of EDTMP and metal ions. An enhanced capacity for adsorption of the modified halloysite toward hydrophilic heavy metal ions would be also shown.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-33**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

3D printing of hydrogel constructs for tissue fabrication

Giho Choi, Kihoon Kim, Minyoung Kim¹, Kwanwoo Shin^{*}

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Bioprinting is a fabrication method for 3D printing of artificial tissues where living cells are encapsulated in biocompatible materials. Unlike the cell seeding on the premade hydrogel scaffolds, bioprinting enables precise positioning of the cells and microvasculature. Microvasculature is a compulsory part of tissue construct since cellular waste and nutrients are removed and supplied through the microvasculature. However, fabrication of hydrogel constructs with micropores or microvasculature is of a challenge since hydrogel inks are difficult to 3D print precisely. Here, we present several methods to 3D print microporous and microvascular hydrogel constructs. In the first approach, sucrose is added in hydrogel ink to increase the viscosity and the printability, as well as to create micropores which function as microvasculature when leached. Another method includes ionic crosslinking of alginate when 3D printed inside the CaCl₂ and Pluronic F127 bath. Pluronic F127 is a shear thinning material which prevents the hydrogel from collapsing during the 3D printing process and is removed afterwards through phase transition. Pluronic F127 can also be used to directly fabricate microvascular structure. Last method includes such microvasculature fabricated by Pluronic F127. Pluronic F127 is 3D printed to make a microvascular structure, and cell-laden hydrogel is poured. When Pluronic F 127 is removed by phase transition, channels devoid of Pluronic F127 function as microvasculature. These methods for fabricating microporous and microvascular structures could improve the material flow between cells and the surrounding hydrogel, promoting the cell viability.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-34**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

3D printing of moldless flexible pressure sensor using bingham plastic

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Devices made from stretchable electronic materials are under huge interest as future application for wearable device in means for clothing or directly attached sensor. Such materials have typically been prepared by engineering elastomeric materials such as silicon.[1] Here we studied 3D printed flexible and moldless fabricated pressure sensor. Stretchable 3D structures were commonly fabricated by mold which are made through complicated process. But by 3D printing the viscoplastic elastomer inside the bingham plastic without mold the structure maintain itself without collapsing. We used CNT/PDMS as piezoresistive nanocomposite to print out pressure sensor structure. The structure is uniformly aligned with independently arrayed deformable pyramidal tips that works as a piezoresistive sensor. The easily deformable pressure sensing tips determines the contact interface, which effects the compressibility in response to external pressure.[2] The counter electrode was easily printed through commercial office printer using silver nanoparticle ink. When the external pressure is introduced, a potential difference with respect to piezoresistive electrode can induce electric current flow through the contact area bridging two terminals. The sensor could sense the continuous and discontinuous finger tapping. Further study through LABVIEW color analysis of pressure distribution with independently arrayed electrodes was also possible. [1] Yamada, T. et al. A stretchable carbon nanotube strain sensor for human-motion detection. *Nature Nanotechnology*. 6, 296-301 (2011) [2] Chwee-Lin, C. et al. Highly stretchable resistive pressure sensors using a conductive elastomeric composite on a micropyramid array. *Advanced Material*. 26, 3451-3458 (2014)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-35**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Solubilization of wrinkle-improving functional materials using nanoparticles

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Development of Drug Development and Discovery, Chungnam National University, Korea

¹*Department of Pharmacy, Korea University Sejong Campus, Korea*

²*Korea Research Institute of Chemical Technology/ M, University of Science & Technology, Korea*

Oleanolic acid, which is used as a major ingredient of medicine and cosmetics separated from various plant species, is an effective ingredient of natural plant and has excellent efficacy against anti-inflammation and stimulation related to skin's physiological activity. In addition, as an anti-aging function, it promotes the synthesis of procollagens, ceramides, filaggins, those which are important for collagen production, and it also has the function of inhibiting the activity of MMP-1, which is an enzyme that destroys polymeric proteins such as collagen. It features a dual anti-aging system that promotes collagen production and prevents destruction. Although Oleanolic acid has a anti-wrinkle function, the low solubility in aqueous solution makes it difficult to be applied as an functional cosmetic material. In this study, the biocompatible polymer is used to solubilize oleanolic acid to remedy the poor solubility. The permeation study was processed for 24 hours using Franz cell to confirm skin permeation rate, and the particle size was analysed by ELS-Z particle analyser. Samples were kept in 40°C for 3 months to confirm long term stability of the nanoparticle. As a result of this study, the solubility of oleanolic acid was improved as it was encapsulated with biocompatible polymers. The skin permeation rate of produced nanoparticle was 15% while rate of control group was 9%. The nanoparticle size was suitable ranging 20-150nm. Nanoparticle was uniform in size and there was no precipitation occurred during long term stability test. This results show that oleanolic acid nanoparticle is expected to be greatly useful in functional cosmetic as an anti-wrinkle material. 본 연구는 미래창조과학부 2017 기술이전사업화 과제의 지원을 받아 수행되었으며 이에 감사드립니다.(과제번호 : 2017-01-DD-049)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-36**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of Natural antimicrobial materials encapsulated nanoparticles

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Among the natural substances, mastic, rosin, myrrh and propolis are famous for their antibacterial effect, but they are substances which are not applicable to various products due to low solubility in aqueous solution. In this study, we have developed a material that can be applied to various products by solubilizing those insoluble antimicrobial material as polymer micellar nanoparticles using biocompatible solvents and block copolymer . Nanoparticles based on surfactants are nano-sized particles formed by amphiphilic (hydrophilic / hydrophobic) polymers in aqueous solution. Amphiphilic block copolymers are grouped in an aqueous solution to form hydrophobic regions inside and outside hydrophilic regions. The nanoparticles were prepared by encapsulating a hydrophobic material such as a mastic and rosin inside the micelle. The particle size of the prepared nanoparticles was analyzed using a particle size analyzer (ELS-Z). To confirm stability of nanoparticles, they were stored at 40 ° C and 25 ° C for more than 3 months respectively. The antibacterial effect was confirmed by microbial detection test for aerobic bacteria and fungi. Mastic, and rosin nanoparticles were found to have an optimal size of 100 nm or less, and the nanoparticles did not show large particle changes or precipitation. Antibacterial effect was confirmed by showing that less than 10 CFU / ml of aerobic bacteria and fungi were detected. We are expecting that the nanoparticle made of natural antimicrobial material can be very useful as environmentally friendly antimicrobial agents using natural materials in the future.본 연구는 한국산업기술진흥원 R&D 재발견 사업의 지원을 받아 수행되었습니다 (과제번호:N0002204)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-37**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Catalytic Depolymerization of Polyesters

Taeyang Do, Jeung Gon Kim*

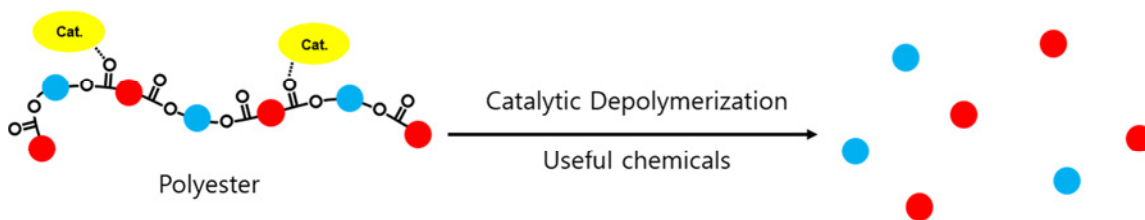
Department of Chemistry, Chonbuk National University, Korea

Polyesters have been used in many applications, but there have been relatively few reports of depolymerization. Rapid and efficient degradation processes using catalysts have also been reported mostly in PET.^[1] We have carried out the depolymerization of various polyester such as Polylactic acid (PLA), Polypropylene carbonate (PCC), Polycarbonate (PC), Polyethylene terephthalate (PET) and Tritan[®]. We tried to show the efficiency of each catalyst using organic and metal complex catalyst used for transesterification. As a result, 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) and 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD), which are organic base catalysts, showed excellent results with high efficiency as known from PET.^[2] Although ZnTAC24[®], a Zn metal catalyst, was inferior to an organic base, it was more reactive than Titanium isopropoxide and Tosylic acid. Both PLA, PCC and PC could decompose under the easier conditions than PET. However, a commercial polymer Tritan[®] is more difficult to decompose due to its poorly soluble properties.

Reference

^[1] N. George, T. Kurian, *Ind. Eng. Chem. Res.*, **2014**, *53*, 14185-14198.

^[2] H. W. Horm, G. O. Jones, D. S. Wei, K. Fukushima, J. M. Lecuyer, D. J. Coady, J. L. Hedrick, J. E. Rice, *J. Phys. Chem. A*, **2012**, *116*, 12389-12398.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-38**

Area: Polymer Chemistry

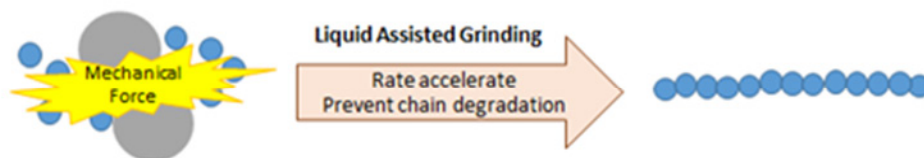
Type: Poster Presentation, Time: FRI 13:00~14:30

Mechanochemical Polymerization of Lactide

NU RI OHN, Jeung Gon Kim *

Department of Chemistry, Chonbuk National University, Korea

The ring opening polymerization (ROP) of lactide has been widely reported.² However, most of the reactions use solvents and metal-catalysts, which are non-green elements. Using ball-mill, we could achieve more environmentally friendly polymerizations.³ The first example of mechanochemical ring opening polymerization of lactide is developed by ball-mill grinding. Mechanical energy from the collision between the balls and the mill beaker effectively promotes an organic based mediated metal- and solvent-free solid state polymerization. Importantly, we have found that the chains degradation, the inherent problem of polymer mechanochemistry, could be solved with liquid assisted grinding (LAG). Liquid assisted grinding accelerates the reaction rate and allows to obtain high molecular weight poly(lactic acid) (> 1 X 10⁵ g/mol) by preventing polymer chain degradation from high energy of ball collision. We also examined frequency and ball effects and it is found that the strength of mechanical energy truly promoted the polymerization. References¹ N. Ohn, J. Shin, S. S. Kim, J. G. Kim, ChemSusChem DOI: 10.1002/cssc.2017008732 Hu, Y., Daoud, W. A., Cheuk, K. K. L., Lin, C. S. K., Materials 2016, 9, 133. James, S. L.; Friščić, T. Chem. Soc. Rev. 2013, 42, 7494-7496.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **POLY.P-39**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Covalent Organic Polymers (COPs) by Natural Aldehyde: Application to the Removal of Heavy Metal Ions from Wastewater

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Covalently bonded organic polymers (COPs) are a new field of functional polymers that have attracted many chemists to date. Because of the comparable surface area, the absence of metal ions in the structure, and the flexibility of molecular design by the synthesis strategy of polymers and organic chemistry, these materials are potential applications for gas separation / storage, heterogeneous catalysts, chemical sensing and heavy metal adsorption. We synthesized COPs which have aminated linkages, constructed by some kind of monoaldehydes and melamine. Our polymers had different BET surface area and pore size distribution. These characteristics of COPs could be controlled by changing the steric effect, and the materials were applied to remove heavy metal ions from wastewater.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-40**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

facile synthesis of xanthate porous polyaminals for heavy metal adsorption

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There is heavy metal contamination is growing as a harmful and hazardous problem on drinking water. Poly(1,3-diphenylurea) were synthesized by schiff-base reaction in DMSO solution and have porosity ranging hierarchically from 0.5~10nm. We expected this polymer can be used for heavy metal removal adsorbent via thiol and carbon disulfide functionalization. In this study, the poly(1,3- diphenylene) will be investigated by BET, ICP-OES, Elemental Analysis, SEM, EDAX for evaluating of heavy metal removal.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-41**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

palladium complex immobilized in porous organic polymer based on urea

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Porous organic polymers (POP) is a material with the great potential to be used in many industries. Due to its large surface area, a lot of research is being carried out in the fields of CO₂ adsorption, catalyst, electrochemical, water treatment and so on. Recently, POP is also used as a catalyst carrier in order to make a heterogeneous catalyst. Heterogeneous catalysts may be lower in catalytic activity than homogeneous catalysts, but are useful in industry because of their ability to be reused. Suzuki reaction is an important reaction in organic chemistry. due to its excellent functional group tolerance, accessibility and the environmental friendly properties of the starting reagents, which are some of the key factors responsible for increased research into this particular reaction. We prepared two POPs based urea group.(UPOP-1, UPOP-2), which was prepared by condensation polymerization of 1,4-phenylene diisocyanate with 1,4-phenylene diamine, melamine, respectively. We evaluate pore structure, structure properties, thermal properties of these POPs by SEM, BET, IR, NMR, TGA. Then we immobilize palladium in these POP for catalytic performance for Suzuki-Miyaura cross-coupling reaction. And evaluated catalytic performance using GC. Acknowledgments This study was supported by the National Research Foundation of Korea (grant no.: NRF-2015R1A4A1042434).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-42**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of thermal expansion capsules with high thermal stability using suspension polymerization

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²*chemical engineering, Inha University, Korea*

Recently, there have been requirements for greater advances in the weight reduction of automotive parts for mileage improvement. In this respect, Thermal Expandable Microsphere (TEM) is a suitable material. They have a core and shell structure. A low-boiling-point hydrocarbon liquid is encapsulated by a polymeric shell. Mixing the microcapsules with the thermoplastic polymer and letting them thermally expand in a polymer can make polymer foams. When the microcapsules are heated to 80~180 °C, they are expanded to 50–100 times greater than their initial volume. In this study, thermally expandable microspheres are synthesized with acrylonitrile (AN) and cyclohexyl methacrylate (CHMA). CHMA is monomer that has high glass transition temperature. So we expected core-shell is expanded on high temperature. Iso-octane and N-octane is used the blowing agent. Suspension polymerization of AN and CHMA initiated by Azobisisobutyronitrile (AIBN). Butanedioldimethacrylate (BDDMA) is used as crosslinker. PVP are used as the Stabilizer. Characterization is used by SEM, TGA, Coulter

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-43**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

3D Printing of Surface Area-controlled Polymeric Structures for As(III) Removal

Kihoon Kim, Giho Choi, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

3D printing which produces objects directly from Computer Aided Designs (CAD) is one of the most versatile and revolutionary technique. 3D printing is a very simple and easy technique to fabricate complex structures which are customized to any personal needs without additional specific tools for the structures. In the meantime, heavy metal pollution has become one of the most serious environmental problems nowadays. Various methods for heavy metal removal including chemical precipitation, ion-exchange, adsorption, membrane filtration and electrochemical methods have their own pros and cons. We fabricated optimized 3D printed polymeric structures for efficient heavy metal removal in the flowing water. These customized polymeric structures are designed to have high surface area coming from specific patterns of structures and modified porous polymeric surfaces. We analyzed the amounts of heavy metal ions in the water are decreased which filtered by these surface area-controlled 3D printed patterns.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-44**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Design of electrochromic polymers for high color contrast with a long bistability

Yeonghwan Heo, younghoon kim, Byeongwan Kim, Eunkyong KIM *

Department of Chemical and Biomolecular Engineerin, Yonsei University, Korea

Conjugated polymers (CPs) show reversible electrochemical optical changes with a high coloration efficiency, which can be applied for external light control such as smart windows, smart sunglasses, and active displays. Among the CPs, Poly(3,4-propylenedioxythiophene) derivatives (PRs) were explored as an electrochromic polymer for high color contrast with long term bistability. To tune HOMO energy level that is critical to bistability of polymers, various functionalized PRs were prepared in three steps. Furthermore, reduce applied potential with same transmittance change with charge balancing layer using TiO₂ nanoparticles. Charge balancing layer can highly improve cycle stability of electrochromic windows. Design principle and electrochromic properties of PRs in a 2-electrode device will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **POLY.P-45**

Area: Polymer Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Preparation of multilayered DMFC membrane by LbL self assembly and click reaction

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Department of Organic And Nano Engineering, Hanyang University, Korea

Multilayered polyelectrolyte membranes were prepared by layer by layer (LbL) self-assembly method. Recently Nafion film is often adopted as membrane for direct methanol fuel cell (DMFC) because of its high thermal stability and proton conductivity, but it also has high methanol permeability which causes decrease of fuel efficiency of DMFC. In this study, polycation(amPSyn) and polyanion(sPSaz) polymers were synthesized and alternately deposited on Nafion substrate to lower methanol permeability of the membrane. Also, to increase the chemical and mechanical stability of the membrane, each polyelectrolyte layer was cross-linked by click reaction. By this method we expect to improve selectivity(proton conductivity/methanol permeability) of the DMFC membrane.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-46**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Synthesis and Characterization of Highly Soluble Scarlet Acid Dyes for Digital Textile Printing

JIEWON 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. Digital textile printing has many advantages as follows. Firstly, It shortens the whole process time due to the elimination of screen plate manufacturing process. Secondly, it is an eco-friendly textile printing process that can reduce the environmental pollution such as waste-water. Finally, It is ideal for short runs, customized designs, and one of a kind prints. In this study, we designed and synthesized four scarlet acid dyes that have high color strength and color purity. We also found the suitable ink formulation recipes in order to apply the synthesized dyes for high-speed DTP. The three scarlet acid dyes were modified from perylene precursors, respectively. The perylene dyes have high tinctorial strength and superior light / heat stability. In order to improve the low water solubility of perylene dyes, sulfonic acid groups were introduced at the bay positions of 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.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: IND.P-47

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

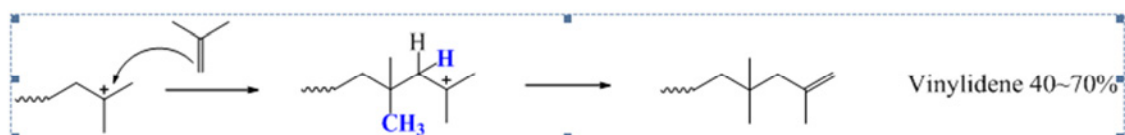
Synthesis of Mid-range Vinylidene Content Polyisobutylene by Using BF₃/N-Propanol Catalyst

Min Sup Park, Yeong-Joon Kim^{1,*}

Department of Chemistry, Chungnam National University / Daelim Industrial Co. SCT, Korea

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

Mid-range vinylidene content polyisobutylenes were prepared by using a Friedel-Craft type catalyst. The polyisobutylenes with 40 to 70% of vinylidene content were obtained when a complex catalyst composed of n-propanol as a cocatalyst and BF₃ as a main catalyst was used at a reaction temperature of -33 to 33° C under a pressure of 3 to 50 kg/cm². The vinylidene contents were easily varied by adjusting the reaction temperature.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-48**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Physical properties analysis of ophthalmic materials with high, medium and low moisture content

Min-Jae Lee, A-Young Sung*

Department of Optometry, Daegu Catholic University, Korea

This study was planned considering the high-, medium-, low-water content materials to be used in the polymerization, while various additives with similar water contents were manufactured. For the preparation of hydrogel ophthalmic lens materials, based of hydrogel ophthalmic lens monomer used in the presence of HEA (hydroxyethyl acrylate), PVP (polyvinylpyrrolidone), NMV were used as additives for preparing the high-water content lens group, and HPMA (hydroxypropyl methacrylate) and BD were used for the medium-water content lens group. For the low-water content lens group, BMA (butyl methacrylate), BDDA (1,4-butanediol diacrylate), and Bis-GMA (bisphenol A glycerolate diacrylate) were used, respectively, at about 10% ratios. The measurements of the contact angles, showed a different wettability value for each lens with a similar water content. And also, the lens curvature according to the change of time showed that the change amount became larger and the recovery time became longer from the lens samples with a lower water content to those with a higher water content. Based on this study, it can be concluded that wettability or other physical properties may be different even though it is a ophthalmic hydrogel lens having a similar water content.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-49**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Characterization of dental resin cement material with antibacterial and high bonding strength

Duck Hyun Kim, Hui-Su Jung¹, A-Young Sung*

Department of Optometry, Daegu Catholic University, Korea

¹*Korea Optics Technology Institute, Korea*

In this study, to manufacture dental resin cement, Bis-GMA and HPMA were used as a major ingredient, camphoroquinone was used as a photoinitiator, TEGDMA was used as a diluent. And also, 2-isocyanato ethyl methacrylate was added to increase the bonding strength and 3-hydroxy pyridine was used as an additive for antibacterial property. The mixture made in accordance to the predetermined ratio was stirred for 24 hours and was polymerized at a wavelength of 440 to 480 nm for 40 seconds. It is considered that this material will be highly applicable as a dental resin cement with high quality.

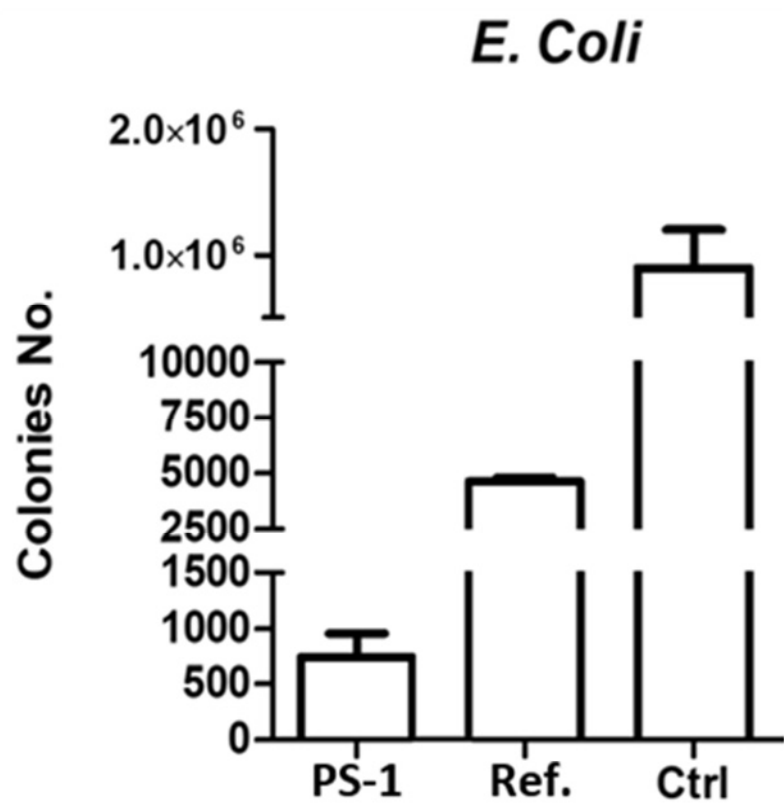


Fig 1. Antibacterial performance of samples.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-50**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Effect of oxyfluorination on pull-out behavior of carbon-fiber-reinforced epoxy matrix composites

Yoon-Ji Yim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

To improve the interfacial adhesion between carbon fibers and an epoxy matrix, carbon fibers were modified by oxyfluorination at different temperature conditions. Surface analyses of the oxyfluorinated carbon fibers were performed using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and dynamic contact angle measurements. The interfacial shear strength (IFSS) of a single carbon fiber/epoxy matrix was studied by employing single-fiber pull-out tests to confirm the interfacial adhesion. The pull-out behavior of the fiber from the matrix was discussed based on the Greszczuk's geometrical model. Functional groups such as C-F, C-O, and COOH were present on the carbon fiber surfaces after oxyfluorination. Moreover, the presence of functional groups increased the surface polarity of the fibers, resulting in an increase in the IFSS owing to the improvement of the interfacial adhesive strength between the carbon fibers and the epoxy matrix.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-51**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electromagnetic Interference Shielding Effectiveness of Metal-plated CNTs/High-density Polyethylene Composites

Yoon-Ji Yim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Multi-walled carbon nanotubes (MWCNTs) were nickel (Ni)-plated chemically to enhance the electromagnetic interference shielding effectiveness (EMI-SE) of Ni-MWCNTs/High-density polyethylene composites (Ni-MWCNTs/HDPE). The surface properties of the Ni-MWCNTs were characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). The EMI-SE of the Ni-MWCNTs/HDPE was tested by a EMI shielding analyzer. The EMI-SE of Ni-MWCNTs/HDPE was enhanced compared to that of as-received MWCNTs/HDPE. Our results indicate that the Ni-MWCNTs can lead to a EMI-SE improvement due to the EMI adsorption behavior of the nickel particles.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-52**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Removal of elemental mercury by activated carbons impregnated with halides

Yoon-Ji Yim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Activated carbons (ACs) were impregnated with potassium halides (KX) to enhance the removal efficiency of elemental mercury (Hg^0). In this work, the impregnation effect of potassium bromide (KBr) and potassium iodine (KI) were investigated. The surface properties of KX-ACs were determined by scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The pore structures and total pore volumes of the KX-ACs were analyzed using the $\text{N}_2/77\text{ K}$ adsorption isotherms. The Hg^0 removal efficiency of KBr-ACs and KI-ACs was studied under simulated flue gas conditions. The effects of KI and KBr loading, adsorption temperature, and flue gas components on Hg^0 removal efficiency were also investigated. The results showed that the Hg^0 removal efficiency of the ACs was significantly enhanced by KI or KBr impregnation, and KI-ACs showed higher Hg^0 removal efficiency than KBr-ACs under the same conditions. An increase in KI or KBr loading and higher adsorption temperatures improved the Hg^0 removal efficiency, indicating that chemisorption occurred due to the reaction between X^- and Hg^0 . The lower extent of Hg^0 removal exhibited by the KBr-ACs than by the KI-ACs was due to the difficulty of Br_2 formation on the surfaces.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-53**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A facile ultrasonic-assisted fabrication of carbon nitride/carbon dots composites for photocatalytic degradation behaviors of rhodamine B

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The novel visible light-induced carbon nitride/carbon dots (g-C₃N₄/CDs) composites were successfully synthesized by introducing CDs into polymeric g-C₃N₄. The structures and optical properties of composites were characterized by XRD, FT-IR, SEM, TEM, DRS, respectively. For the degradation of rhodamine B (Rh B), the g-C₃N₄/CDs composites exhibited significantly higher visible light photocatalytic activity than that of a single semiconductor. The optimal percentage of CDs was 50%. In addition, the stability of the prepared composites in the photocatalytic process was also investigated. The enhanced photocatalytic performance could be due to the high separation efficiency of the photogenerated electron–holes pairs. The possible photocatalytic mechanism of g-C₃N₄/CDs was proposed to guide the further improvement of their photocatalytic activity.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-54**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

In-situ synthesis of BiOCl_x/BiOBry/BiOIz nanofibers for visible-light photocatalytic investigation

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In this work, BiOCl_x/BiOBry/BiOIz/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/BiOIz/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/BiOIz 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.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-55**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

In-situ growth of Graphene Oxide/BiOCl composites 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 photogenerated electron and holes between BiOCl and graphene oxide, and the better adsorption capacity of rhodamine B.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-56**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile synthesis of nitrogen-doped microporous carbons derived from microporous imine-linked polymer for efficient CO₂ adsorption

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Department of Chemistry, Inha University, Korea

Microporous organic polymers containing heteroatoms are considered as promising substrates for CO₂ capture and separation with a tangible effect on the atmosphere and clean energy applications. In the present work, we have reported a cost-effective strategy for designing a series of carbonized products by high-temperature treatment of an imine and benzimidazole linked polymer (IBLP). The resulting materials exhibit a high surface area with narrow micropores. CO₂ adsorption measurements reveal a notable uptake capacity up to 130.4, 98.4, and 87.5 mg/g at 273, 298, and 308 K, respectively, along with the high isosteric heats of adsorption (30.4 - 32.2 kJ/mol). Presence of micropores and heteroatom in the solid adsorbents with the high thermal stability accompanied with excellent CO₂/N₂ selectivity proclaimed the nitrogen-enriched carbon as promising candidates for CO₂ scrubbing technology.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-57**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Designing microporous carbons from melamine-based polyaminals for carbon dioxide adsorption

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Heteroatom doping and well-tuned porosity are considered as significant factors of porous carbon materials for various applications. However, it is still challenging to tune a single variable while retaining the other factors unaffected, which limits rational and systematic research. In this work, in situ nitrogen-doped porous carbon materials were prepared by direct pyrolysis of conjugated microporous polymer precursors with the same skeleton structure. It was found that the CO₂ adsorption capability was significantly enhanced compared with their precursors due to the optimized pore configuration. Thus, this work provides a valuable insight into the design and preparation of high performance materials for CO₂ capture and energy storage applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-58**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile synthesis of microporous carbonaceous materials through Schiff base polymer for CO₂ capture

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Department of Chemistry, Inha University, Korea

Highly porous nitrogen-doped carbon materials were synthesized by the carbonization of a low-cost porous covalent Schiff-base polymer synthesized by the reaction of readily available monomers. The nature of the bond and structure of the resulting materials were confirmed using various spectroscopic methods, and the effects of activation on the textural properties of the porous carbon materials were also examined. The activated porous carbon materials possessed a high surface area and large micro/total pore volumes with narrower micropore size distributions. The fabricated sorbents exhibited the best CO₂ uptakes which are comparable to the performance of some benchmark carbon materials under the same conditions. The prepared materials exhibited high CO₂ /N₂ selectivity and could be regenerated easily.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-59**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study of nanodiamond/nitrile-butadiene rubber nanocomposites fabricated by one-pot design

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3-Mercaptopropyltrimethoxysilane (MPTMS)-ethanol solution treated nitrile butadiene rubber/nanodiamond (NBR/ND) polymer nanocomposites were prefabricated in-situ by a novel environmentally friendly one-pot design. The nanodiamond (ND) and modified nanodiamond (MND) were characterized by using wide angle X-ray diffraction (WAXD), Fourier transformation infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), an adsorption analyzer (BELBELSORP), thermal gravimetric analysis (TGA), and X-ray photoelectron spectroscopy (XPS). The results show that the pristine ND is provided not only with high specific surface area, but also with abundant active organic groups, especially hydroxyl and carboxyl groups, which confirms the hydrophilic properties of nanodiamond. The morphology of the fracture surfaces of NBR/(M)ND nanocomposites are studied by high resolution scanning electron microscopy (HR-SEM). The dynamic rheological properties of NBR/(M)ND nanocomposites were characterized by rubber processing analyzer (RPA). The NBR/MND composites exhibited superior mechanical property attributing to the stronger interfacial interaction via covalent bonding between MND and NBR molecules compared to the NBR/ND composites that connected by weaker π - π stacking.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-60**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Rheological behavior of mercapto-terminated silane-treated rice bran carbon/nitrile butadiene rubber composites

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The surface morphology and structure of novel rice bran carbon (RBC) were characterized by X-ray diffraction, thermogravimetric analysis, high-resolution scanning electron microscopy (HR-SEM), Raman spectroscopy, and adsorption analysis. The RBC/nitrile butadiene rubber (NBR) polymer-matrix composites were fabricated by using the latex compounding technique, based on the superior hydrophilic characteristics of RBC. The covalent bonding process was conducted by in situ interfacial modification technique. The dispersion of RBC and the interfacial morphologies between the RBC and NBR matrix were confirmed by HR-SEM. The bonding mechanism was analyzed in detail by mechanical and dynamic rheological determinations. At the same filler concentration, the MPTMS treated composites exhibited stronger mechanical properties than original RBC/NBR composites, as the interfacial interaction via MPTMS connected RBC and NBR molecules was stronger than the interaction in NBR/RBC composites connected by hydrogen bonds and weaker π - π stacking.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-61**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Simple preparation of sponge-like graphene-based carbon frameworks by non-template method for electrodes of supercapacitor

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Sponge-like graphene oxide/carbon nanotubes (S-GO/CNT) composites were prepared by integrating GO nanosheets and CNT via non-template method. The as-prepared S-GO/CNT composites possess highly holey structure, leading to providing highly effective electrolyte pathway. Reduced S-GO/CNT (rS-GO/CNT) which can be used as electrode in supercapacitor can be prepared by annealing the S-GO/CNT composites without distinct deformation. The characterization of S-GO/CNT and rS-GO/CNT composites was investigated by X-ray diffractometer, transmission electron microscope and scanning electron microscope. The electrochemical measurements of rS-GO/CNT composites were performed by cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The rS-GO/CNT electrode possesses excellent rate capability and cycling stability owing to its high electrical conductivity and superior structural stability.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-62**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Nanodiamond nanocluster decorated-graphene oxide for fabricating epoxy nanocomposites

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Hybrid fillers composed of nanodiamond (ND) decorated graphene oxide (GO) were incorporated into epoxy matrix with a novel thermoregulatory liquid-liquid extraction method. Energy dispersive spectroscopy, X-ray diffraction spectroscopy, Fourier transform infrared and X-ray photoelectron spectroscopy analysis confirmed chemical bonding between the 3-aminopropyltriethoxysilane functionalized nanodiamond (ND-APTES) and 3-Glycidoxypropyltrimethoxy silane functionalized graphene oxide (GO-GMPTS). The morphology of the hybrid filler, GN was characterized by high-resolution transmission electron microscopy. ND nanoclusters with an average diameter of 50-100nm were uniformly grown on the GO surface. The hybrid filler provided significant enhancement of mechanical properties, such as flexural strength, flexural modulus and impact strength. In particular, the epoxy composites containing 0.1wt% hybrid GN exhibited a higher mechanical behavior compared to the one containing 0.2 wt% GO.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-63**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study on polymerization properties of polyethylene wax with metallocene catalyst

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In this study, we have studied characterization of metallocene catalysts used for polymerization of polyethylene wax. 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. We have also checked hydrogen used for chain transfer agent, molecular weight change and distribution by different ratios of ethylene gas. Finally, we suggest proper structure of metallocene catalysts for polymerization of polyethylene wax.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-64**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Prediction of the diffusion coefficient for infinite water based on quantitative structure-property relationship modeling

YE-EUN KIM, Byeong Hun Lee, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

In physical chemistry, the diffusion coefficient is the amount of material that diffuses from one space to another under constant conditions of volume and concentration, and is the area of each cross-sectional unit per unit time. This is one of the important parameters used in diffusion, distillation, adsorption, and chemical reaction processes of various fields. The factors affecting the diffusion coefficient of chemicals are the bond types, the melting point, the crystal structure of the diffusing material, the presence of the medium and the temperature. In this study, quantitative structure-property relationship models were developed for predicting diffusion coefficient for infinite water from 2D chemical structure. The experimental diffusion coefficients from 5000 compounds at 298 K were collected for model development. In the 556 predefined descriptor pools, a suitable descriptors for learning model was pre-filtered. Learning method for linear and non-linear fitting was performed using multiple linear regression and support vector machines. Also Y-scrambling test was performed to verify that chance correlation of the models and the confidence range of the model were defined as kNN-based applicability domain. These models can predict the diffusion coefficient limit for infinite water and new compounds.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-65**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of predictive QSPR model of octanol-air partition coefficient for pollutants

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The octanol-air partition coefficient (KOA) is invaluable for predicting the extent to which a substance partitions from the atmosphere to environmental organic phases such as organic constituents of soil, vegetation, aerosol particles, and even indoor carpet. Also this is useful for assessing chemical transport and persistence of chemicals, which are required by regulatory agency to evaluate new and existing chemicals. In this study, we developed QSPR models for predicting KOA, which their data were collected from literatures. 717 KOA data were divided into training set and external test set, and molecular descriptors were calculated from 2D chemical structure using the PreADMET program. As it is important to select essential features from a large number of molecular descriptors to develop a robust and predictive QSPR model, we compared two kinds of feature selection method the population based forward selection(PBFS) and the genetic algorithm(GA). Multiple linear regression(MLR) and support vector machine(SVM) were used as learning algorithm to develop QSAR model. The chance correlation and predictability of these model were validated by y-scrambling method and external validation. The reliable range of prediction model can be identified from the kNN based applicability domain(AD).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-66**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

New Solid State Photochemistry of Siloles Driven by ortho-Carborane: Insight on Structure-Property Relationships

Hyun Wook Cha, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Regioisomeric silole-carboranes, Si-*p*-Cb and Si-*m*-Cb, were prepared. As incorporating ortho-carboranes onto the silole, their emissions in solution state were quenched due to the electron transfer from silole core to the ortho-Cb groups. Furthermore, Si-*p*-Cb and Si-*m*-Cb showed different photophysical properties. In THF solution, even though their emissions were weak, Si-*p*-Cb reveals competitive radiative process from local excited state and charge transfer state which produced dual emissions at 480 nm and 570 nm, while Si-*m*-Cb showed emission from LE state at 480 nm. Most interesting features of regioisomeric silole-carboranes were found in their solid state photochemistry. In amorphous phase, Si-*p*-Cb showed strong emission at 570 nm along with weak emission at 480 nm while Si-*m*-Cb showed single emission at 480 nm. In crystalline phase, on the other hand, major radiative process for Si-*p*-Cb was changed to LE state which showed hypsochromic shift to 480 nm. Completely reversed phenomenon was observed for Si-*m*-Cb which showed bathochromic shift to 570 nm in crystalline phase. Namely, CT states of regioisomeric Si-Cb can be turn-on or turn-off depending on substitution positions. This phenomenon was explained by variation of dihedral angles between silacyclopentadiene ring and phenyl rings at 2- and 5-positions. When they are in orthogonal positions, electronic communications between silole ring and ortho-carborane groups are retarded which results dominant emission from LE state, which refers CT state is turn-off. On the other hand, when they are in horizontal position, CT state is turn-on and reveals CT emission. Namely, small modification on their substitution position changed their excited state properties and results different radiative processes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-67**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis, and Photophysical Properties of Blue Phosphorescent Heteroleptic Iridium(III) complexes

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A series of heteroleptic Ir(III) complexes composed of 2-(2,4-difluoro-3-(trifluoromethyl)phenyl)-4-methylpyridine (dfCF₃) as the main ligand and such ancillary ligands as acetylacetonate [Ir(dfCF₃)₂(acac)] (acac), picolinate [Ir(dfCF₃)₂(pic)] (pic), and tetrakis-pyrazolyl borate [Ir(dfCF₃)₂(bor)] (bor) were prepared, and their emission behaviors depending on the ancillary ligands were systematically investigated. It was found that the Huang–Rhys factors (SM_s) of the emission decrease in the order bor (0.97) > acac (0.87) > pic (0.76), while the nonradiative rate constants (k_{nr}/10⁵ s⁻¹) calculated from the quantum yields and lifetimes of emission were in the order acac (4.89) > pic (1.17) > bor (0.28). It was assumed that the large difference of k_{nr} for the complexes arose from important contributions of the ancillary ligands to the crossing from an emissive state (³MLCT) to a nonemissive metal-centered state (³MC). The activation energies for the crossing from ³MLCT to ³MC were estimated from the temperature dependencies of the emission lifetime and were found to be 46 meV for acac, 61 meV for pic, and > 100 meV for bor. The experimental results were in line with the theoretical calculations based on integrating quantum chemical modeling methods. By the excellent emission behavior, bor was applied as a dopant to prototype deep-blue phosphorescent organic light-emitting diode devices, which revealed high emission efficiency and colour purity.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-68**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Investigation of the Electrochemical, Photochemical, and Spectroelectrochemical Properties of the Ir (III)/Pt (II) and Ir(III)/Ir(III) Bimetal Complex bridged by Dipyridylpyrazine

Bo-Sun Yun, Yang-Jin Cho, So-Yoen Kim, DAE WON CHO, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

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We investigated the electrochemical and excited-state properties of 2,3-bis(2-pyridyl)pyrazine (dpp)-bridged bimetallic complexes, (L)₂Ir-dpp-PtCl (1, L = 2-(4',6'-difluorophenyl)pyridinato-N,C₂ (dfppy); 2, L = 2-phenylpyridinato-N,C₂ (ppy)) and [(L)₂Ir]₂(dpp) (3, L = dfppy; 4, L = ppy) compared to monometallic complexes, (L)₂Ir-dpp (5, L = dfppy; 6, L = ppy) and dpp-PtCl (dpp-Pt^{II}Cl₂) (7). The same L (C^N) ligand exhibited close similarities in their electrochemical, photophysical, photochemical, and transient absorption decay behavior. The similarities were: potentials of the dpp^{0/-}, dpp⁻²⁻, and L^{0/-} couples in CV, the absorption spectra with similar spectral shape and absorption coefficients, the emission spectra at 77 K similar in wavelength and lifetime, the complete or extensive quenching of emission at room temperature, and the selective photochemical splitting of the metal-dpp linkages. The lowest-energy absorption and emission is attributed by L(π)-participated MLCT transitions occurring between the (L)₂Ir-based orbitals and dpp-localized π* orbital. The low efficiencies of photoluminescence of dpp-bridged Ir-Pt and Ir-Ir bimetallic complexes (1–4) could be explained by assuming the involvement of crossing to Pt- and Ir-based d-d states from the emissive state. The crossing to such d-d states has been assumed to be thermally accessible as a consequence of the strained planar conformation of dpp that should give impacts on relative energy levels of the relevant d-d states in the bimetallic complex.

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Code: **IND.P-69**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Detailed Investigation of Photophysical Properties of Isomeric Carbene Ir(III) Complexes and their Applications to Deep-blue Phosphorescent Organic Light Emitting Diodes

JaeHyun Park, Yang-Jin Cho, So-Yoen Kim, Jin-Hyoung Kim, Won-Sik Han¹, Sang Ook Kang, Ho-Jin Son*

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We synthesized two isomeric N-heterocyclic (NHC) carbene Ir(III) complexes, *f*-Ir-(dbfmi)₃ (1) and *m*-Ir-(dbfmi)₃ (2), and the photophysical and electrochemical properties of the compounds were investigated. Both isomers showed efficient emission in dichloromethan solution with quantum yield 53% and 68%, respectively, arising from the unusual properties of the N-heterocyclic carbene (NHC) ligand—that is, the complexes possess a strong metal–ligand bond that destabilizes the non-radiative metal–centered ligand-field states. Depending on their configurations, they showed different photophysical properties which reveal that the emission of facial isomer is relatively dominance of ³LC state while meridional isomer shows significant ³MLCT character. Furthermore, emission lifetime of both isomers were gradually increase in rigid environment which indicates their efficiencies can be improved when they utilized in OLEDs. Accordingly, both isomeric complexes were used as dopant material for blue PHOLED device. Both devices showed high efficiencies with EQE of up to 18% and low turn-on voltage (≈ 2.8 V). Most importantly, device with *m*-Ir-(dbfmi)₃ showed deep blue CIE chromaticity diagrams with (0.14, 0.11).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-70**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Important role of some ancillary ligand in Blue Phosphorescent Iridium(III) Complexes with Sulfonyl-Substituted ligand

Jin-Hyoung Kim, DAE WON CHO, Sang Ook Kang, Ho-Jin Son*

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A series of heteroleptic Ir(III) complexes composed of 3-(pyridin-2-yl)benzene-1-sulfonyl fluoride (SO_2F) as the main ligand and such ancillary ligands as acetylacetonate [$\text{Ir}(\text{SO}_2\text{F})_2(\text{acac})$] (acac), picolinate [$\text{Ir}(\text{SO}_2\text{F})_2(\text{pic})$] (pic), and tetrakis-pyrazolyl borate [$\text{Ir}(\text{SO}_2\text{F})_2(\text{bor})$] (bor) were prepared, and their emission behaviors depending on the ancillary ligands were systematically investigated. Phosphorescence origin of the sulfonyl group has been studied and emissive ^3LC and $^3\text{MLCT}$ were found to be directly related to emission quantum yield as well as emission color. Within the context to delineate the sulfonyl group effect, emission properties of the ancillary ligands have been scrutinized by means of emission photo-kinetics: a blue-shift emission is observed on going from acac ($\lambda_{\text{max}} = 490 \text{ nm}$) to bor ($\lambda_{\text{max}} = 460 \text{ nm}$). Density-functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were employed to investigate the geometries, electronic structures and photophysical properties of three phosphorescent Ir(III) complexes. Elaboration of the sulfonyl group effect will be fully disclosed by the photodynamic studies and its significant role will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **IND.P-71**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Spectroscopic study on the phosphorescence of Pt-complexes

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In order to understand the relation between the narrowing of emission band and structural changes, we synthesised tetradentate Pt-complexes; Pt-1 has directly connected two carbazole (Cz) moieties, Pt-2 has additional two methyl groups to Pt-1, and Pt-3 is one Cz moiety. The absorption and emission spectra of Pt-1 are identical with those of Pt-2. The emission of Pt-3 observed at shorter wavelength compared to others. The 0-0 vibronic band of all Pt-complexes was quite intense compared to the 0-1 vibronic band, which may due to the restricted structure of tetradentate ligand. The spacing of 0-0 and 1-0 vibronic bands are 1487 and ~ 1323 cm^{-1} . To determine the cause of this spacing, we have carried out the theoretical study using the DFT calculation and the analysis of IR-spectra. Also, we have carried out transient Raman experiment to get the vibronic informations of excited Pt-1. We achieved the narrow-band emission from Pt-complexes using tetradentate ligand, and we have evaluated the origin of shoulder vibration band in emission spectra.

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Code: **IND.P-72**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Tuning steric and electronic effects in phosphorescent Ir complex with terphenyl-modified phenylimidazolate unit for Blue Organic Light-Emitting Diodes

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Department of Advanced Materials Chemistry, Korea University, Korea

Six new cyclometalated iridium complexes of terphenyl-modified phenylimidazolate ligands (tpim) were synthesized and characterized in order to examine the effect of bulky substituents on the structure-property relationship of these iridium complexes. Introducing bulky groups on the phenylimidazole ligand can effectively block the transition of nonradiative 3MC state and improve the emission lifetime. In order to demonstrate the bulkiness effect, X-ray single crystal structure analysis and theoretical quantum chemistry calculations were performed, and photophysical and electrochemical measurements were carried out. These results indicated that the terphenyl-phenylimidazolate iridium complexes have potential application in fabrication deep-blue phosphorescent organic light-emitting diode devices.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-73**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Novel compounds having Ceramide structure and it's application

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Ceramide is present in the outer layer of skin and enhanced internal barriers from outside the skin and protect skin and hair. However, it is difficult to apply easily because not easily obtainable. Research on ways to make ceramide more cost-effective is ongoing. Research on ways to improve high-cost and bad solubility issues. Ceramide structure has devised that can improve performance and solubility. And we successfully synthesised. Synthesis of Ceramide we used alkyl amine and succinic anhydride, and solvent was used. The structural analysis was conducted through NMR analysis, and the LC-MSMS analysis was confirmed thermal stability. Performance assessment was performed by dividing skin and hair. The skin was measuring in moisturizing ability. Measurements were made at the same time as checking the electrical conductivity and Transepidermal water loss And The hair has been evaluated such as strength, friction, and breakage. A comparative evaluation of the synthesised Ceramide and previously known ceramide was performed. Our synthesised ceramide Performance was confirmed superior, and solubility also confirmed superiority. The ceramide keeps the skin barrier and protects from the outside environment and keeps the moisture outflow from the barrier. In the hair, it was found that ceramide inserted between the cuticle and the strength of the hair improved, as the adhesive It is expected that the scope of the application will be significantly wider. because we solve bad solubility and high-cost issues. Continuous tracking tests should be conducted on reliability and safety. Not only for body, but also the products they eat are being released. If you can understand the depth of Ceramide, it is believed that you will benefit greatly from Ceramide.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: IND.P-74

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Important Role on Intermolecular Charge Transfer and Photoinduced Electron Transfer by π -conjugation in D- π -A and D- π -Si- π -A dyads

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In order to elucidate the influence of π -conjugation on photoinduced electron transfer (PET) and intramolecular charge transfer processes, donor- π -acceptor dyads (D- π -A (1) and D- π -Si- π -A (2)), were newly synthesized. In these molecules, triazine and carbazole moieties acted as the electron acceptor and donor, respectively. The photoluminescence of 1 red-shifted with increase of solvent polarity. In the excited state of 1, the π -conjugation acted as the linker for charge transfer ($D^{\delta+}$ - π - $A^{\delta-}$) between the donor and acceptor moieties. The changing of a large dipole moment ($\Delta\mu=45.6$ D) between the ground and excited states was determined using the Lippert-Mataga plot. In case of 2, the π -conjugation is disconnected by a Si-atom in the linker. The fluorescence of 2 showed weak dual-emission: a short-wavelength emission at around 350 nm arising from the monomeric species and a long-wavelength one assigned to the emission from an intramolecular exciplex between the donor and acceptor moieties: the $D^{+\cdot}$ - π -Si- π - A^{\cdot} was generated by PET process in the excited state. Each radical species was verified by an fs-TA investigation. We conclude that the disconnection of π -conjugation between the donor and acceptor causes a unit-electron transfer rather than a partial charge transfer. In this case, the linker cannot contribute as a part of the chromophore. In an NLO (nonlinear optical) process such as two-photon absorption, the perturbation between the donor and acceptor demands the π -conjugation of the linker.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **IND.P-75**

Area: Industrial Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Prediction on the thermal properties of the castable plastic bonded explosive using the thermal analysis data

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In the PBXs(Plastic Bonded Explosives),thermal property is important characteristic. Through the thermal analysis data, it can predict the thermal properties of Plastic Bonded Explosives.To analyze the thermal property of PBXs, there are various methods and tools. Differential Scanning Calorimetry(DSC) and accelerated rate calorimeter are a typical method for thermal analysis not only for common chemicals but also energetic materials. In the dynamic DSC measurements, thermodynamic change of castable PBXs such as melting interfere kinetic evaluation. So isothermal or Heat-Wait-Search method are often performed to avoid thermodynamic issues. In this study, we report prediction of properties for castable PBXs using AKTS kinetic program through thermal calorimeter measurements.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-1**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Shape and Composition Effects of Palladium Catalysts for Ethanol Oxidation Reaction

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Polymer electrolyte membrane fuel cells (PEMFCs) have attracted interests due to high efficiency, environment-friendly and low electrode reaction temperature compared other cells. Palladium (Pd) catalysts have significant properties at ethanol oxidation reaction (EOR) of anode fuel oxidation reaction in PEMFCs. Controlling shape and composition of Pd catalysts at nanoscale enhances electrocatalytic activity. Notably, size and crystallinity of catalysts can influence on their catalytic activities due to modification of surface area and energy. In addition, optimization of binding strength between surface atoms of Pd catalysts and molecules can be obtained by control of composition ratio. Herein, we have synthesized two shapes of palladium nanoparticles of cube and octahedron and sulfidation of pre-formed palladium nanoparticles for using a facile synthesis method. Measuring scanning electron microscopy (SEM) and transmission electron microscopy (TEM) compared shapes of palladium and palladium sulfide nanoparticles and cyclic voltammetry (CV), electrocatalysis properties of palladium catalysis in ethanol oxidation reaction as anode half-cell.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-2

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

**Crystal structure of inorganic-organic hybrid perovskite type
(C₆H₅CH₂CH₂NH₃)₂ZnCl₄ by X-ray single crystal diffraction:
Comparison with (C₆H₅CH₂CH₂NH₃)₂CoCl₄ and
(C₆H₅CH₂CH₂NH₃)₂ZnBr₄**

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As a part of the interest in the low-dimensional magnetism, we synthesized a series of inorganic-organic hybrid perovskite type materials whose general chemical formula is (C₆H₅CH₂CH₂NH₃)₂MeX₄ where Me = divalent metal and X = halides [1, 2]. Depending on the type of the transition metals, each crystal shows completely different crystal systems and magnetic behavior. For example, Co-PEA crystallized in P2₁/c and shows no magnetic transition and in the crystal structure, Co²⁺ cation builds an isolated tetrahedron with four Cl⁻ anions [1]. Contrary to Co-compound, Mn- and Cu-PEA crystallized in the same space group Pbc_a and each transition metal is surrounded by six Cl⁻ anions. However, Mn-PEA shows an antiferromagnetic phase transition at 43K and Cu-PEA has a Curie temperature at 10K [2, 3]. Zn-PEA belongs to the monoclinic space group P2₁/c with a = 7.455Å, b = 24.67Å, c = 11.203Å and β = 91.71°. These values are very similar to Co-PEA (P2₁/c with a = 7.462Å, b = 24.664Å, c = 11.997Å and β = 91.76°) and also Zn-bromide (C₆H₅CH₂CH₂NH₃)₂ZnBr₄ system (P2₁/c with a = 7.67Å, b = 25.53Å, c = 11.14Å and β = 91.40°) [1, 4]. In this work, we will compare Zn-chloride system with Co-chloride and Zn-bromide systems from a crystal structural point of view.

Reference

- [1] I. H. Oh et al., Acta Cryst. E, 67 (2011) m522.
- [2] S. H. Park et al., Dalton Trans., 41 (2012) 1237.
- [3] A. O. Polyakov et al., Chem. Mater., 24 (2012) 133.

[4] Y. D. Huh et al., CAP, 6 (2006) 219.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-3

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Photophysical and electron accepting properties of multi-*o*-carboranylbenzene compounds

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Multiple *o*-carborane substituted compounds, mono-, 1,3-bis-, and 1,3,5-tris-(2-(4-butylphenyl)-*o*-carboran-1-yl)benzene (**1–3**) were prepared and characterized by multinuclear NMR spectroscopy and elemental analysis. The solid-state structures of **2** and **3** were also verified by single crystal X-ray diffraction. While the monocarborane compound **1** was non-emissive in solution state at 298 K, the photoluminescence (PL) spectra of **2** and **3** showed weak to moderate emission ($\lambda_{em} = 352$ nm for **2** and 363 nm for **3** in THF). Compounds **2** and **3** exhibited intriguing dual emission bands ($\lambda_{em} = 361$ and 537 nm for **2** and $\lambda_{em} = 387$ and 520 nm for **3**) at 77 K and in film, of which the low-energy band was main in the solid state. TD-DFT calculations on the S_1 optimized structures suggested that the low-energy fluorescence of **2** and **3** was attributed to the $\pi(4\text{-butylphenyl}) \rightarrow \pi^*(\text{phenylene-}o\text{-carborane})$ intramolecular charge transfer (ICT) transition. The low-energy electronic transition of **2** and **3** was obviously associated with an aggregation-induced emission (AIE), and enhanced emission intensity ($\lambda_{em} = \text{ca. } 570$ nm for **2** and $\lambda_{em} = \text{ca. } 550$ nm for **3**) was observed upon increasing the water fraction (f_w) in THF/water mixtures. Furthermore, the PL experiments of poly(3-hexylthiophene-2,5-diyl) (P3HT) polymer films doped with **3** revealed the excellent electron-accepting properties of **3**.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-4

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Photophysical changes of Biphenylene Based *o*-Carboranyl Compounds by Distortion of Biphenyl Rings

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Four biphenyl- and fluorene-based *o*-carboranyl compounds, **1B**, **2B**, **1F**, **2F**, were prepared and characterized by multinuclear NMR spectroscopy and elemental analysis. The crystal structures of **1B** and **2B**, analyzed by single-crystal X-ray diffraction, exhibited distinct distortions of the central biphenyl rings with dihedral angles of 44.2 and 33.1°. In photoluminescence measurements, fluorene-based carboranyl compounds in the rigid state (e.g., in solution at 77 K and as films) exhibited a obvious emission in the low-energy region below 400 nm. **1F** displayed a low-energy emissive trace in solution at ambient temperature, whereas biphenyl-based carboranes mainly exhibited high-energy emissions above 400 nm. TD-DFT calculations on the first excited singlet (S_1) state of each compound suggested that the emission in the low-energy region involves intramolecular charge transfer (ICT) between the carborane and central phenylene rings, indicating that the radiative decay of these ICT bands could be enhanced by preventing the distortion of the central biphenyl groups. Furthermore, less distortion on the biphenyl rings of the biphenyl-based analogues at S_1 in the optimized structures supports that these phenylenes must be level for the formation of stable excited states. Comparison of the quantum efficiency (Φ_{PL}) and radiative decay constants (k_r) of the *o*-carboranes also reveals clearly that the structural features of the biphenyl groups can have a decisive effect on those photophysical properties.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-5

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ratiometric emission change by deboronation of 1,3,5-tris-(*o*-carboranyl-methyl)benzene

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The detection of fluoride anions, contributes in the protection of the environment. Although fluoride is necessary in dental health-care and in the prevention and treatment of osteoporosis at optimum concentrations, it is considered a biohazard at high concentrations. In this regard, receptors or reactants that can bind with fluoride anions have been actively studied for their potential in the development of chemosensors. 1,3,5-Tris-(*o*-carboranyl-methyl)benzene (*closo-1*) and its *nido*-form (*nido-1*) were synthesized and completely characterized. The solid-state molecular structure of *closo-1* was determined by single-crystal X-ray diffraction analysis. Compound *closo-1* showed a great single emission in various organic solvents that was bathochromic shifted with increasing solvent polarity. The positive solvatochromic effect and theoretical calculation results at the first excited (S_1) optimized structure of *closo-1* strongly propose that this emissive band can be assigned to an intramolecular charge transfer. Meanwhile, *nido-1* showed a noticeable bathochromic shift of the emissive band compared to that of *closo-1* and aroused low-energy emission. The specific emissive aspects of *nido-1* were attributed to the elevation of its HOMO level, estimated by cyclic voltammetry. The photophysical changes by conversion from *closo-1* to *nido-1* allowed the emissive color-tunable sensing of fluoride. Thus, the tris-*o*-carboranyl compound exhibited great potential as a chemodosimeter for fluoride anion sensing, detectable by the naked-eye.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-6**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Unprecedented Reactivity of Copper(II)-Alkylperoxo Complexes in Aldehyde Deformylation

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Copper(II)-alkylperoxo adducts, $[\text{Cu}(\text{CHDAP})(\text{OOR})]^+$ (CHDAP = N,N'-dicyclohexyl-2,11-diaza[3,3](2,6)pyridinophane; R = C(CH₃)₂Ph and ^tBu), were prepared and characterized by various physicochemical methods such as UV-vis, CSI-MS, resonance Raman and EPR. These are the first synthetic Cu(II)-alkylperoxo complexes that can perform aldehyde deformylation (i.e., nucleophilic reactivity) under the stoichiometric reaction conditions, which was confirmed by kinetic studies. Moreover, the metastable Cu(II)-alkylperoxo complexes are able to catalyze C-H bond activation through O-O bond cleavage at higher temperature.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-7**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Metal compound filters for disposal of hazardous materials

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Metal compounds containing zirconium were investigated as effective filters for disposal of hazardous materials such as chemical warfare agents. The filters were fabricated as a circular disk and the zirconium compounds can include $Zr(OH)_4$, ZrO_2 , and $C(CH_3CO_2)_xZr(OH)_y(x+y \sim 4)$. Of particular, $Zr(OH)_4$ effectively absorbed sulfur mustard (HD) and released nontoxic chemicals as products. To increase the catalytic effect of zirconium compounds, the whole sample was heated at moderately elevated temperatures of 100 °C. The products of degradation were directly transferred and analyzed by FT-IR and GC-MS. As reference, MgO was used, which showed no effective degradation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-8

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ortho Donor-Appended Triarylboron Emitters for Record-High Efficiency in Pure Blue TADF Organic Light-Emitting Diodes

Young Hoon Lee, SURENDRAN SUJITH, HeeChai Lee, Jung Jaehoon, Min Hyung Lee*

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Highly efficient thermally-activated delayed fluorescence (TADF) is proposed using ortho donor (D)—acceptor (A) compounds (PXZoB, DPAoB, CzoB) wherein acceptor is based on triarylboron and donor is phenoxazine (PXZ), diphenylamine (DPA), or carbazole (Cz). Combined with the ortho D—A connectivity, the bulky nature of the triarylboron endows the D—A dyads with inherent steric “locking” for highly twisted arrangement, leading to a small energy difference between singlet and triplet excited states (ΔE_{ST}) and thus exhibiting very efficient TADF with microsecond-range lifetimes. In sharp contrast, the corresponding para D—A derivatives, DPApB and CzpB, only display short-lived, normal fluorescence. Organic light-emitting diodes (OLEDs) incorporating the proposed ortho D—A compounds as emitters display orange, greenish-blue, and pure blue emission, and exhibit high external quantum efficiency (η_{EQE}). In particular, the pure blue OLEDs based on the proposed ortho D—A emitters with a carbazole donor (CzoB) shows the record-high η_{EQE} of 22.6% with CIE color coordinates of (0.139, 0.150), well illustrating the validity of the proposed approach. Upon optical optimization, its η_{EQE} is further improved to 24.1%.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-9**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Turn-On Fluorescence Sensing of Fluoride Ion by Donor-Antimony(V) Lewis Acids

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Fluoride sensing has been an important topic during the last decade because of the detrimental effect of fluoride in physiological systems. In particular, detection of fluoride at low concentrations, such as the parts per million level, in aqueous media has been an important issue from a practical point of view. In recent years, organoantimony(V) Lewis acid compounds are attracting growing interest due to their high binding affinity towards fluoride anion in both organic and aqueous media as well as turn-on fluorescence response upon fluoride complexation. In this work, a series of donor-Sb(V) stibonium compounds has been prepared bearing donor as 10H-phenoxazine (3a), diphenylamine(3b), and carbazole (3c) to investigate the change in photophysical properties upon fluoride binding. These stiboniums are almost nonemissive, but their fluorostiboranes display donor-centered fluorescence due to the locally excited $\pi\pi^*$ state. The carbazole donor containing compound (3a) exhibits the most intense turn-on fluorescence response toward fluoride binding with a high binding constant ($K > 10^7 \text{ M}^{-1}$) in MeCN. Details of synthesis, characterization, and photophysical properties of Sb(V) stibonium compounds will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-10**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Manipulating the Number of *o*-Carboranyl Ligands of Iridium(III) Cyclometalates for the Improved Photophysical and Electroluminescent Properties

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A series of iridium(III) cyclometalates with mono-, bis-, and tris-*o*-carboranyl ligands, *fac*-[m-(2-MeCB)ppy]_nIr(ppy)_{3-n} (n = 1–3, m = 5 (3a-5a); m = 4 (3b-5b); 2-MeCB = 2-methyl-*o*-carboran-1-yl; ppy = 2-phenylpyridinato-C²,N), was prepared to investigate the impact of the number of *o*-carboranyl ligands on the photophysical and electroluminescent properties. While the phosphorescence wavelengths of 3a-5a and 3b-5b were blue-shifted or red-shifted with respect to that of *fac*-Ir(ppy)₃ (6), respectively, both series underwent gradual hypsochromic shifts as the number of carboranyl ligands was increased. All of the complexes exhibited moderate to high phosphorescence quantum efficiencies in toluene and the quantum efficiency increased as the number of carboranyl ligands increased. Solution-processed green phosphorescent organic light-emitting diodes (PhOLEDs) incorporating the 5-substituted complexes (3a-5a) as emitters exhibited a similar level of high performance, of which the best performance was observed for devices based on 4a. Furthermore, vacuum-deposited devices were successfully fabricated with mono- and bis-carboranyl complexes, 3a and 4a. The resulting devices showed excellent performance, which was improved by ca. 40% compared to those of the solution-processed devices.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-11**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Strategic Design of 2,2'-Bipyridine Derivatives to Modulate Metal-Amyloid- β Aggregation

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The complexity of Alzheimer's disease (AD) stems from the inter-relation of multiple pathological factors upon initiation and progression of the disease. To identify the involvement of metal-bound amyloid- β (metal-A β) aggregation in AD pathology, among the pathogenic features found in the AD-affected brain, small molecules as chemical tools capable of controlling metal-A β aggregation were developed. Herein, we report a new class of 2,2'-bipyridine (bpy) derivatives (1–4) rationally designed to be chemical modulators toward metal-A β aggregation over metal-free A β analogue. The bpy derivatives were constructed through a rational design strategy employing straightforward structural variations onto the backbone of a metal chelator, bpy: (i) incorporation of an A β interacting moiety; (ii) introduction of a methyl group at different positions. The newly prepared bpy derivatives were observed to bind to metal ions [i.e., Cu(II) and Zn(II)] and interact with metal-A β over metal-free A β to varying degrees. Distinguishable from bpy, the bpy derivatives (1–3) were indicated to noticeably modulate the aggregation pathways of Cu(II)-A β and Zn(II)-A β over metal-free A β . Overall, our studies of the bpy derivatives demonstrate that the alteration of metal binding properties as well as the installation of an A β interacting capability onto a metal chelating framework, devised via the rational structure-based design, were able to achieve evident modulating reactivity against metal-A β aggregation. Obviating the need for complicated structures, our design approach, presented in this work, could be appropriately utilized for inventing small molecules as chemical tools for studying desired metal-related targets in biological systems.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-12**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Unprecedented nitrile reactivity mediated by a peroxocobalt(III) intermediate

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Oxidation processes mediated by metal-dioxygen adducts have attracted much attention in biomimetic and enzymatic reactions. Although a number of metal-dioxygen species have been prepared and investigated in oxidation reactions with diverse organic substrates under mild conditions, reactivities with nitriles have rarely been explored. Herein, we report that a side-on peroxocobalt(III) complex with a tetradentate macrocyclic ligand shows a novel and facile mode of dioxygenase-like reactivity with acetonitrile to give a mononuclear hydroximatocobalt(III) complex in which the nitrile is oxidized by two oxygen atoms of the peroxo group. ¹⁸O labeling experiments confirm that both oxygen atoms are derived from the peroxo ligand. This unprecedented mode of nitrile reactivity was also seen for other nitriles, e.g., CH₃CH₂CN and C₆H₅CN, each of which gives the corresponding hydroximatocobalt(III) complexes. Kinetic studies including the Hammett analysis and isotope labeling experiments suggest that this novel mode of nitrile activation occurs via a concerted mechanism. This new reaction will significantly expand the range of nitrile activation processes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-13

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and properties of dinuclear Pd(II) and Pt(II) complexes bearing a bridged π -conjugated group

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Dinuclear Pd(II) and Pt(II)-halides bearing bridged π -conjugated groups, trans,trans-[(PR₃)₂(X)M-Ar-M(X)>(PR₃)₂] (M = Pd, Pt; X = Cl, Br; ArH₂ = terpyridine, fluorenone, benzyl, benzthiadiazole) were prepared from the double oxidative addition of dihalo- π -conjugated moieties (6,6'-dibromo-2,2':6',2''-terpyridine; 2,7-dibromo-9-fluorenone; 4,4'-dibromobenzil, 4,7-bis(2-bromo-5-thienyl)-2,1,3-benzthiadiazole) to the Pd(styrene)(PR₃)₂. In addition, when the dihalosilole derivatives (2,5-dibromo-1,1-dimethyl(or diphenyl)-3,4-diphenylsilole) reacted with Pd(styrene)(PR₃)₂, mono or dinuclear Pd(II) complexes bearing the dimethyl(or diphenyl)-3,4-diphenylsilole group were obtained. The obtained compounds were characterized by spectroscopic and elemental analyses. π -Conjugated extension reactions of dinuclear Pd(II) halides bridged by bithiophene group with HC≡C-R {R = SiPh₃, C(O)OMe } in the presence of CuI and HNEt₂ caused the selective formation of bis(acetylide) Pd(II) complexes, Pd(C≡C-R)₂(PR₃)₂ and bithiophene. Experimental details will be discussed.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-14**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and catalytic properties of *cis*-(*R*)- (BINAP)bis(azido)palladium(II)

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New Pd(II) azido complex bearing (*R*)-BINAP (2,2'-bis(diphenylphosphino)-1,1'-binaphthyl), which was prepared from reaction of the corresponding (BINAP)PdCl₂ with excess NaN₃, examined chemical property toward organic isothiocyanate to afford S-coordinated tetrazole-thiolato Pd(II) compounds. Also, the catalytic C-C coupling reactions using *cis*-(*R*)-(BINAP)bis(azido)palladium(II) were carried out.

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Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-15

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Stepwise Synthesis and Selective Sensing of Nitrobenzene Using Copper(I) Coordination Polymers

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Five Copper(I) coordination polymers (CPs), $[\text{Cu}_2\text{I}_2\text{L}_2]_n$ (**1**), $[\text{Cu}_4\text{I}_4\text{L}_2]_n$ (**2a**), $\{[\text{Cu}_4\text{I}_4\text{L}_2] \cdot 2\text{CH}_3\text{CN}\}_n$ (**2b**), $\{[\text{Cu}_4\text{I}_4\text{L}_4] \cdot 0.5\text{C}_6\text{H}_6\}_n$ (**2c**), $\{[\text{Cu}_6\text{I}_6\text{L}_2] \cdot 2\text{C}_3\text{H}_6\text{O}\}_n$ (**3**) have been prepared by self-assembly reactions between CuI and 2-(2-benzylthio)ethylpyrazine (L). CPs **1-3** are determined by single crystal x-ray diffraction. CPs **1** and **3** were crystalized in space group orthorhombic *Pbca* and monoclinic *P2₁/n*, respectively. CPs **2a-2c** were crystalized in space group triclinic *P-1*. CP **1** has a 2D network structure based on dimer-like Cu_2I_2 cluster nodes and CPs **2a-2c** have 1D loop chain structures based on stair step-like Cu_4I_4 cluster nodes, in which solvent molecules are different. CP **3** shows a 2D network structure based on 1D stair-step of stair-step (Cu_6I_6)_n polymers. The solvent-mediated reversible crystal-to-crystal transformations between CPs **2a-2c** were achieved by exposing solvent vapor or soaking the crystalline samples in diverse solvents (acetonitrile, benzene). Interestingly, CP **3** has been stepwisely synthesized from CP **1** via CP **2b** by removal of L, which cannot be obtained by the direct reaction of L and CuI. Moreover, emission of CP **2b** is selectively quenched by nitrobenzene with good sensitivity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-16**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Cu(I) Coordination Polymer Based on Thioether Ligands with Pyridine Dicarboxylic Anhydride

Juhyeon Park, Hyunjin Park, Hansu Im, Tae Ho Kim^{*}, Myong Yong Choi^{*}

Department of Chemistry, Gyeongsang National University, Korea

The ligands (**L**¹, **L**², **L**³ and **L**⁴) with thioether substituents were synthesized by the reaction of pyridine dicarboxylic anhydride and 2-(cyclohexylthio)ethylamine or 2-(tert-butylthio)ethylamine. One Cu(I) coordination polymer (CP) $\{[\text{Cu}_4\text{I}_4\text{L}_2] \cdot \text{MeCN}\}_n$ (**1**) was prepared by the reaction of CuI and **L**². CP **1** showed a 1D loop chain structure based on cubane Cu₄I₄ cluster nodes. CP **1** was crystalized in space group triclinic *P*-1. Remarkably, CP **1** is non-emissive at room temperature in comparison with most emissive cubane Cu₄I₄ complexes. The results of our investigation including syntheses, structural characterization, thermal properties of one new Cu(I) coordination polymer is presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-17

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Reversible Crystal Transformation between Cubane and Stairstep Cu₄I₄ Clusters of Cu(I) Coordination Polymers Base on a mixed N/S Donor Ligand

Hansu Im, Hyunjin Park, Tae Ho Kim^{*}, Jineun Kim^{*}

Department of Chemistry, Gyeongsang National University, Korea

The copper(I) compounds, [Cu₄I₄L₄] (**1**), [Cu₄I₄L₂MeCN]_n (**2**) and {[Cu₄I₄L₂]·MeOH}_n (**3**), containing a mixed N/S donor ligand, 2-(benzylthio)-N-(pyridin-3-yl)acetamide (**L**) has been synthesized and structurally characterized by single crystal X-ray diffraction analyses. Compound **1**, **2** and **3** were crystallized in the space group tetragonal I4₁/a, orthorhombic Pbca and monoclinic P2₁/n, respectively. Compounds **1** and **3** are composed of cubane Cu₄I₄ cluster nodes. Compound **1** shows a discrete structure, whereas **3** shows a 2D network structure with solvate MeOH molecules. Compound **2** shows a 2D network structure based on stair-step Cu₄I₄ cluster nodes. Remarkably, crystal-to-crystal transformations between **1** and **2** was accompanied by conversion between stair step and cubane Cu₄I₄ clusters by addition of **L** and CuI. Compound **2** was transformed to **3** by addition of methanol and compound **3** was transformed to **2** by exposure of acetonitrile vapor. Therefore, the transformations between supramolecular isomers **2** and **3** are completely reversible.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-18**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nonheme Iron(IV)–Imido versus Iron(IV)–Oxo Complexes

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A mononuclear nonheme iron(IV)-imido complex, $[(13\text{-TMC})\text{Fe}^{\text{IV}}(\text{NTs})]^{2+}$, was generated and characterized by various spectroscopic methods such as UV/vis, EPR, Mössbauer and rRaman. The reactivity studies revealed that the iron(IV)-imido complex is capable of C-H bond activation and nitrene transfer reactions. In H-atom abstraction reactions, based on the observations of the KIE value and the good correlation between the reaction rates and the C-H BDEs of substrates, the H-atom abstraction from the C-H bonds of substrates by $[(13\text{-TMC})\text{Fe}^{\text{IV}}(\text{NTs})]^{2+}$ is the rate-determining step. Reactivity comparison between iron(IV)-oxo and -imido complexes has been discussed in the C-H bond activation and nitrene transfer reactions.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-19**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

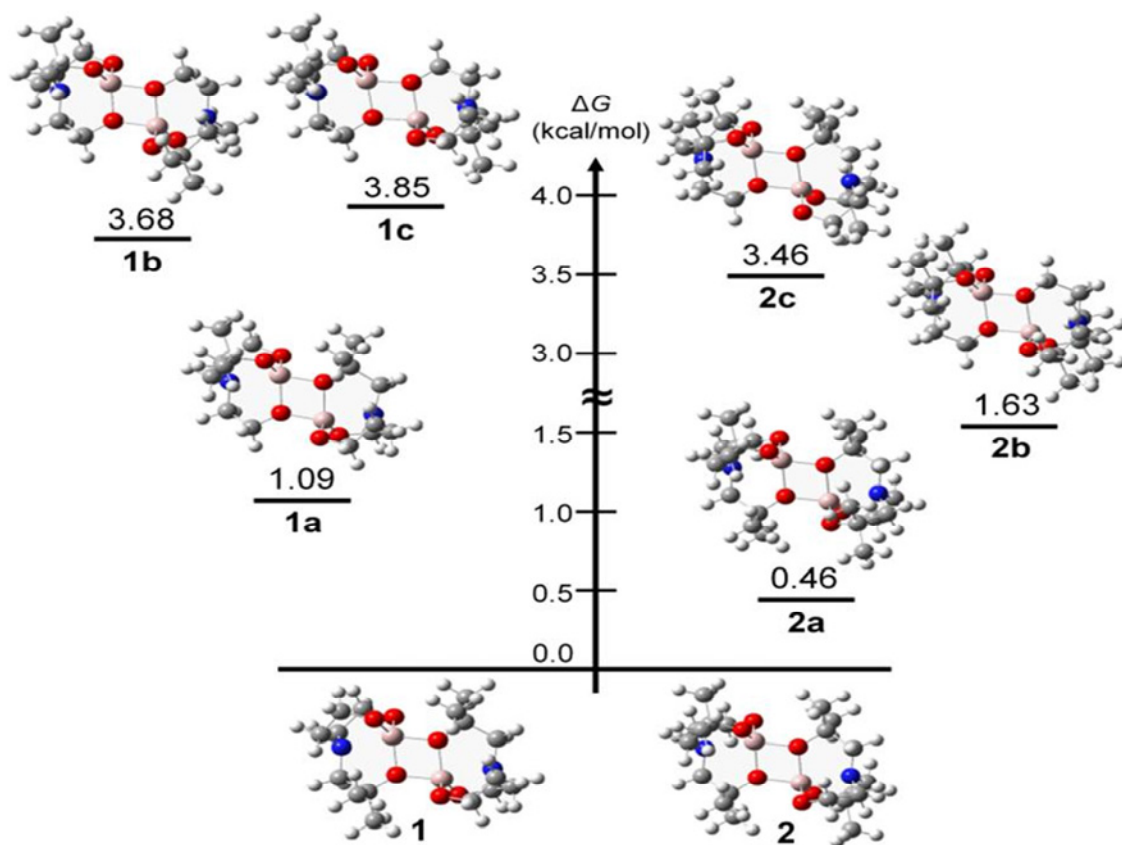
Synthesis of Dimeric Alumatrane with Tricyclic Five-membered Rings and their Usage as Catalysts for Trimethylsilylcyanation Reaction

Yoseph kim, Kang Mun Lee¹, Youngjo Kim^{*}

Department of Chemistry, Chungbuk National University, Korea

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

We designed and explored novel dimeric alumatrane with tricyclic five-membered rings. The obtained alumatrane were all dimeric in the solid state, solution phase, and the gas phase. According to single-crystal X-ray analysis, the first structurally characterized dimeric alumatrane abnormally had their sterically bulky side arms with dimethyl substituents in the bridging sites of the tetradentate ligand, which was also determined by DFT calculations. The new alumatrane were used as catalysts for the trimethylsilylcyanation reaction of aldehydes under extremely mild conditions of room temperature, less than 0.5 mol% catalyst loading, and a short reaction time of 1 h. The new catalytic systems showed high catalytic activities regardless of the aldehyde type, which included electron-rich, neutral, and deficient aryl aldehydes, heterocyclic aldehydes, and alkyl aldehydes. Figure 1. Computed free energy diagram for possible alumatrane isomers. **ACKNOWLEDGMENT:** This work was supported by the National Research Foundation of Korea (NRF), the Korean Ministry of Education (MOE) through the Creative Human Resource Training Project for Regional Innovation (grant number 2014H1C1A1066874).



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Code: **INOR.P-20**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Metallacyclodimeric Array Containing Both Channels and Cages: Photoluminescence Recognition of Diiodomethane

Jeong Jun Lee, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of ZnX_2 ($X = Cl, Br, \text{ and } I$) with 2,3-bis(4'-nicotiamidophenoxy)naphthalene L as a hemi-circular bidentate ligand containing chromophore moiety yields a systematic 46-membered metallacyclodimeric unit, $[ZnX_2L]_2$. These basic skeletons constitute, via interdigitated $\pi \cdots \pi$ interactions in a staggered fashion, a unique ensemble forming both channels and cages. This can then be employed as an unusual "small molecule-recognition within the channel and the cage" host-guest system. Specifically, the ensemble with channel and cage significantly stabilizes the CH_2I_2 molecules in the order $[ZnI_2L]_2 > [ZnBr_2L]_2 > [ZnCl_2L]_2$. These three complexes have significant halogen effects on the photoluminescence (PL), thermal properties, and host-guest inclusion. The unprecedented supra ensemble containing both channel and cage reversibly adsorbs/desorbs small solvent molecules.

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Area: Inorganic Chemistry

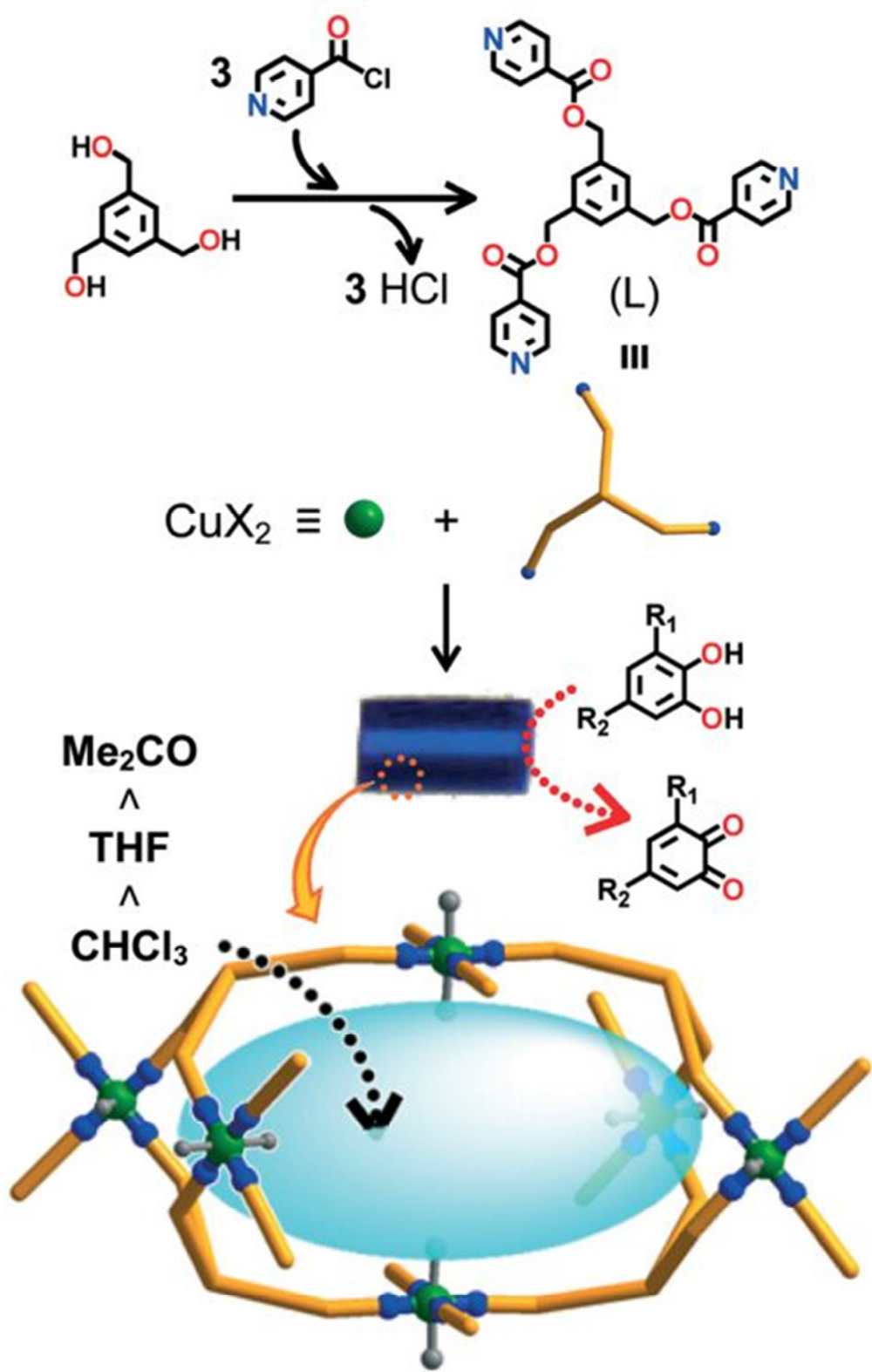
Type: Poster Presentation, Time: THU 11:00~12:30

Catechol oxidation catalysis and solvent inclusion of 3D copper(II) coordination networks

Daseul Lee, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

The reaction of CuX_2 ($\text{X}^- = \text{ClO}_4^-$ and BF_4^-) with a new 1,3,5-tris(isonicotinoyloxymethyl)benzene (L) ligand gives rise to 3D coordination networks, $[\text{Cu}_3\text{L}_4(\text{CH}_3\text{CN})_6](\text{X})_6$, with a new topology of the Schläfli point symbol $\{4 \cdot 8^2\}_4\{4^2 \cdot 8^2 \cdot 10^2\}_2\{8^4 \cdot 12^2\}$. $[\text{Cu}_3\text{L}_4(\text{CH}_3\text{CN})_6](\text{ClO}_4)_6$ and $[\text{Cu}_3\text{L}_4(\text{CH}_3\text{CN})_6](\text{BF}_4)_6$ networks have useful oval-shaped pores of $11.2 \times 11.2 \times 24.8 \text{ \AA}^3$ and $11.1 \times 11.1 \times 24.4 \text{ \AA}^3$ dimensions, respectively. These porous coordination networks act as good heterogeneous catalysts, oxidizing the catechols in the order 3,5-di-tert-butylcatechol (3,5-DBuCat) > 4-tert-butylcatechol (4-BuCat) > 4-chlorocatechol (4-ClCat). The catalytic effect of $[\text{Cu}_3\text{L}_4(\text{CH}_3\text{CN})_6](\text{BF}_4)_6$ is slightly higher than that of $[\text{Cu}_3\text{L}_4(\text{CH}_3\text{CN})_6](\text{ClO}_4)_6$. The pores of the 3D networks reversibly adsorb the solvents in the order chloroform > tetrahydrofuran > acetone.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-22**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation and Catalytic effect of zinc(II) 3D coordination networks

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Self-assembly of $\text{Zn}(\text{ClO}_4)_2$ with 1,1,2,2-tetramethyl-1,2-di(pyridin-3-yl)disilane (L) as a bidentate N-donor gives rise to 3D coordination networks, $[\text{Zn}(\mu\text{-OH})(\text{L})]_3(\text{ClO}_4)_3 \cdot 5\text{H}_2\text{O}$ ($1 \cdot 5\text{H}_2\text{O}$), of unique, 103-*asrs* net topology. An important feature is that two enantiomeric 3D frameworks, 41- and 43- $[\text{Zn}(\mu\text{-OH})(\text{L})]_3(\text{ClO}_4)_3 \cdot 5\text{H}_2\text{O}$, are interpenetrated to form a racemic two-fold 3D network with cages occupied by two water molecules. Another structural characteristic is a C₃-symmetric planar $\text{Zn}_3(\mu\text{-OH})_3$ 6-membered ring with tetrahedral Zn(II) ions. The steric hindrance of substrates and trace water effects on transesterification catalysis using the network have been scrutinized. The coordination network acts as a remarkable heterogeneous transesterification catalytic system that shows both the significant steric effects of substrate alcohols and momentous water effects. The substrate activity is in the order ethanol > *n*-propanol > *n*-butanol > *iso*-propanol > 2-butanol > *tert*-butanol. For the reaction system, solvate water molecules within the cages of the interpenetrated 3D frameworks do not decrease the transesterification activity, whereas the trace water molecules in the substrate alcohols act as obvious obstacles to the reaction. Reference [1] E. Choi, M. Ryu, H. Lee and O.-S. Jung, Dalton Transactions, , 2017, 46, 4595

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-23

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Unusual Rigid 2D Topology of Copper(II) Complexes Effects On Catechol Oxidation

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Department of Chemistry, Pusan National University, Korea

The self-assembly of CuX_2 ($\text{X}^- = \text{Cl}^-, \text{Br}^-, \text{NO}_3^-, \text{ClO}_4^-, \text{and } \text{BF}_4^-$) with a new diallylbis(pyridin-3-yl)silane ligand (L) gives rise to the similar 2D coordination networks with composition of Cu(II) and L of 1 : 2 irrespective of anions and solvents. The 2D networks of $[\text{CuCl}_2\text{L}_2] \cdot 2\text{H}_2\text{O}$, $[\text{CuBr}_2\text{L}_2] \cdot 2\text{H}_2\text{O}$, and $[\text{Cu}(\text{H}_2\text{O})_2\text{L}_2] \cdot (\text{NO}_3)_2$ are packed in a staggered mode while the similar networks of $[\text{Cu}(\text{BF}_4)_2\text{L}_2]$ and $[\text{Cu}(\text{ClO}_4)_2\text{L}_2]$ are arrayed in a eclipsed fashion. These crystals of all 2D networks have been employed as catalysts for 3,5-di-tert-butylcatechol (3,5-DBCat) oxidation, showing the catalytic effects in the order of $[\text{CuCl}_2\text{L}_2] \cdot 2\text{H}_2\text{O} > [\text{CuBr}_2\text{L}_2] \cdot 2\text{H}_2\text{O} > [\text{Cu}(\text{H}_2\text{O})_2\text{L}_2] \cdot (\text{NO}_3)_2 > [\text{Cu}(\text{ClO}_4)_2\text{L}_2] > [\text{Cu}(\text{BF}_4)_2\text{L}_2]$ in chloroform and exhibiting the catalytic effects of only $[\text{Cu}(\text{H}_2\text{O})_2\text{L}_2] \cdot (\text{NO}_3)_2$ in acetone. Thus, the catalytic effect on catechol oxidation is strongly dependent on anions and media.

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Code: **INOR.P-24**

Area: Inorganic Chemistry

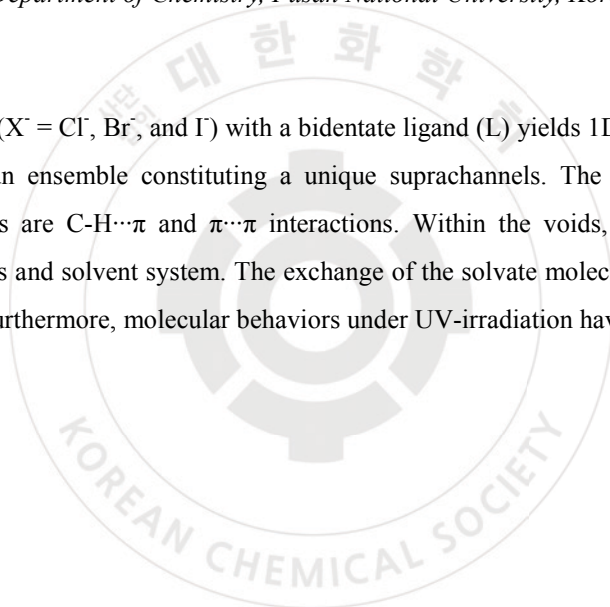
Type: Poster Presentation, Time: THU 11:00~12:30

Construction and photoreaction of 1D Zn(II) suprachannels

Haeri Lee, Ok-Sang Jung*

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Self-assembly of ZnX_2 ($X^- = Cl^-, Br^-, \text{ and } I^-$) with a bidentate ligand (L) yields 1D zigzag-chains, $[ZnX_2L]$. The 1D chains form an ensemble constituting a unique suprachannels. The main driving forces for suprachannel ensembles are $C-H \cdots \pi$ and $\pi \cdots \pi$ interactions. Within the voids, solvate molecules exist depending on the anions and solvent system. The exchange of the solvate molecules in a crystalline solid state was carried out. Furthermore, molecular behaviors under UV-irradiation have been investigated.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-25**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fluorescence Quenching Effect using Sandwich Shape Zn(II) Complex Containing Trisilane Ligand

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Self-assembly of $Zn(ClO_4)_2$ with 1,3,5-tris(dimethyl(pyridin-3-yl)silyl)benzene (L) as a new C_3 -symmetric tridentate N-donor gives rise to a discrete sandwich-shaped M_3L_2 architecture, $[Zn_3(\mu-OH)_3L_2](ClO_4)_3 \cdot 4CH_3CN \cdot 2H_2O$. Its blue photoluminescence is significantly quenched only by CH_2I_2 among the various small molecules, CH_2Cl_2 , CH_2Br_2 , $CHCl_3$, 1,2-dichloroethane, EtOH, CH_3CN , benzene, toluene, and phenol. The sandwich-shaped M_3L_2 Zn(II) complex has interesting structural features, and its strong blue photo-luminescence efficiently recognizes the CH_2I_2 molecule. Although the photo-response is still far from suitable for practical applications, the uniquely shaped complex, based on the novel ligand, is promising as a photoluminescent sensor for specific small molecules. According to the results, the fluorescence quenching follows the dynamic quenching mechanism. These results could provide important clues to the design of capsule-like self-assemblies having potential catalyst, sensor, and recognition applications. Additional and more systematic studies, for example on the synthesis and coordination frameworks of related ligands, are in progress.

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Code: **INOR.P-26**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Theoretical Elucidation of Catalytic Borylation of Methane

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

The C–H functionalization of hydrocarbon using Ir catalyst has been studied so far.[1] In particular, C–H bond activation of methane is one of the intriguing challenges because of its stability and inertness. We are, therefore, interested in the catalyst design for methane activation. Recently, we reported the catalytic borylation of methane by combining computational and experimental study.[2] Experimentally, we obtained monoborylated methane with 2–5% yield with Ir(1,10-phenanthroline)(Bpin)₃ (pin = pinacol) catalyst, whereas Ir(dmpe)(Bpin)₃ catalyst generates with 52% yield.[2] Herein, we suggest a suitable mechanism and elucidate the catalytic difference of two catalysts using DFT calculations. The calculation results show that the overall barrier for the Ir(dmpe)(Bpin)₃ is lower than that of Ir(1,10-phenanthroline)(Bpin)₃, which is good agreement with the previous results. In addition, based on HSAB principle, we can explain the catalytic difference between two ligands. References[1] (a) Labinger, J. A.; Bercaw, J. E. *Nature* 2002, 417, 507. (b) Bergman, R. G. *Nature* 2007, 446, 391. (c) Hartwig, J. F. *Acc. Chem. Res.* 2012, 45, 864. [2] Smith, K. T.; Berritt, S.; Gonzalez, M.; Ahn, S.; Smith, M. R. III.; Baik, M.-H.; Mindiola, D. J. *Science* 2016, 351, 1424.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-27**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Simple synthesis of MgCO_3 and $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ through alkali metal nitrate medium

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MgCO_3 and $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ are anhydrous forms of magnesium carbonate, which are hard to synthesize in aqueous solution at ambient temperature and pressure because of large hydration energy of magnesium ion. Molten salt provides liquid medium at higher temperature than normal solvents, enabling the synthesis of various kinds of metal oxides. Furthermore, alkali metal nitrates are frequently used as promoting agents for MgO-based CO_2 absorbent at intermediate temperature (200-500 °C). Based on these backgrounds, we synthesized pure crystalline anhydrous MgCO_3 and $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ by heating hydromagnesite (MCH, $4\text{MgCO}_3 \cdot \text{Mg}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$) and an alkali metal nitrate at 325 °C under CO_2 flow. Water of hydration decomposes and $\text{Mg}(\text{OH})_2$ reacts with CO_2 to form MgCO_3 at given condition. The existence of Na_2CO_3 determines the products being MgCO_3 or $\text{Na}_2\text{Mg}(\text{CO}_3)_2$. Every kind of alkali metal nitrate successfully acted as a reaction medium, giving different particle morphology. The characterization of samples were performed by powder X-ray diffraction measurements (XRD), thermogravimetric analyzer (TGA), and field emission scanning electron microscopy (FE-SEM), which verified that the synthesized products are pure anhydrous rhombohedral MgCO_3 and $\text{Na}_2\text{Mg}(\text{CO}_3)_2$.

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Code: **INOR.P-28**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Tuning the Redox Reactivity of a Nonheme Iron(III)-Peroxo Species by Binding Redox-Inactive Metal Ions

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Redox-inactive metal ions are one of the most important co-factors involved in dioxygen activation and formation reactions by metalloenzymes. In this presentation, we have shown that the rate constants of electron transfer and C-H bond activation reactions by nonheme iron(III)-peroxo complexes binding redox-inactive metal ions, $[(14\text{-TMC})\text{Fe}^{\text{III}}(\text{O}_2)]^+-\text{M}^{\text{n}+}$ ($\text{M}^{\text{n}+} = \text{Sc}^{3+}, \text{Y}^{3+}, \text{Lu}^{3+}, \text{and La}^{3+}$), increases proportionally with the increase of the Lewis acidity of the redox-inactive metal ions (ΔE). In contrast, the rate constants of the $[(14\text{-TMC})\text{Fe}^{\text{III}}(\text{O}_2)]^+-\text{M}^{\text{n}+}$ complexes in nucleophilic reactions with aldehydes decreases proportionally as the ΔE value increases. Thus, the Lewis acidity of the redox-inactive metal ions bound to the mononuclear nonheme iron(III)-peroxo complex modulates the reactivity of the $[(14\text{-TMC})\text{Fe}^{\text{III}}(\text{O}_2)]^+-\text{M}^{\text{n}+}$ complexes in electron-transfer, electrophilic, and nucleophilic reactions.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-29**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Mechanistic Insights in Postsynthetic Ligand Exchange of Metal-Organic Frameworks

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Department of Chemistry, Chungbuk National University, Korea

Metal-organic frameworks (MOFs) are solid material consisted by coordination bonds between metal clusters (e.g., secondary building units, SBUs) and organic linkers.^[1] Recently, it was revealed that the coordination bonds between SBU and carboxylic acid on MOFs is in dynamics, and the exchange phenomenon was successfully applied to 'functionalization methods' for MOFs. Both cations and ligands could be incorporated into MOF structures, and several experimental data supports this observation follows the exchanges process and not dissolution/re-aggregation process.^[2,3]

In this presentation, our recent studies about postsynthetic ligand exchange (PSE) on a zirconium-based MOF, UiO-66 (UiO = University of Oslo) with some mechanistic clues will be presented. We have examined that target ligand effects, parent MOF effects, and structural defect effects to obtain the mechanistic evidence for PSE. In addition, the sequential PSEs were performed to prepare multi-layer type or core-shell type MOFs with three different ligands. The detail preparation methods for ligand and PSE procedures will be discussed along with kinetic data.

References

- [1] H.-C. Zhou, J. R. Long, O. M. Yaghi, *Chem. Rev.*, **2012**, *112*, 673.
- [2] M. Kim, J. F. Cahill, Y. Su, K. A. Prather, S. M. Cohen, *Chem. Sci.* **2012**, *3*, 126.
- [3] M. Kim, J. F. Cahill, H. Fei, K. A. Prather, S. M. Cohen, *J. Am. Chem. Soc.* **2012**, *134*, 18082.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-30**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Functional Group Controls in Zr-MOFs for Xe/Kr Separation

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Among the various MOFs (metal-organic frameworks), group IV metal, a zirconium-based MOF, UiO-66 (UiO = University of Oslo), is considered to be one of the most chemically and physically stable MOFs. Using their superior stability, a variety application has been reported including catalysis and industrial applications. And, moreover, Zr-MOF has recently been shown to be a good candidate for adsorptive separation of Xe/Kr mixtures. Since the ability to impart chemical functionalities is an attractive characteristic of MOFs, herein, we prepared a series of functionalized UiO-66 materials (UiO-66-NH₂, UiO-66-(OMe)₂, UiO-66-NH₂(OMe)₂, and UiO-66-F₄) by incorporating pre-synthesized several polar functionalities into UiO-66 framework.

We found that a series of electron-rich and electron-deficient UiO-66 materials have stronger interactions with Xe and Kr atoms than pristine UiO-66. We also found that Xe/Kr selectivity increases with the electron density of the ligand. Among the series of UiO-66s, UiO-66-NH₂(OMe)₂ exhibited the highest Xe/Kr Henry's constant ratio (14.4), possibly due to having the highest electron density as well as an unsymmetrical arrangement of functional groups of the ligands. The detail synthetic procedure of ligands and MOFs also will be presented.

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Area: Inorganic Chemistry

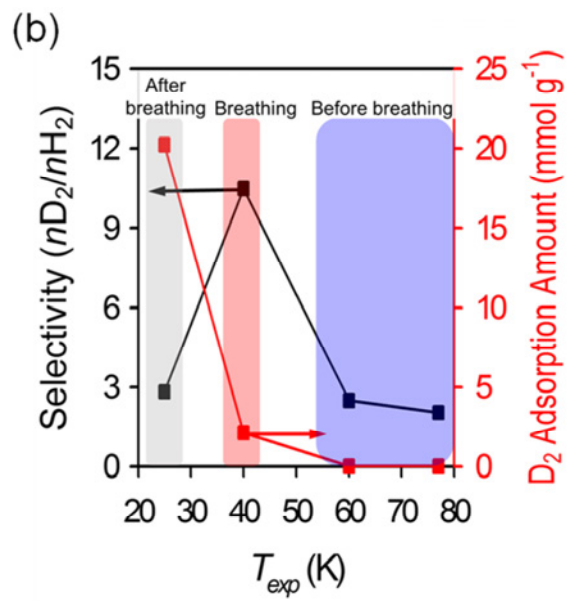
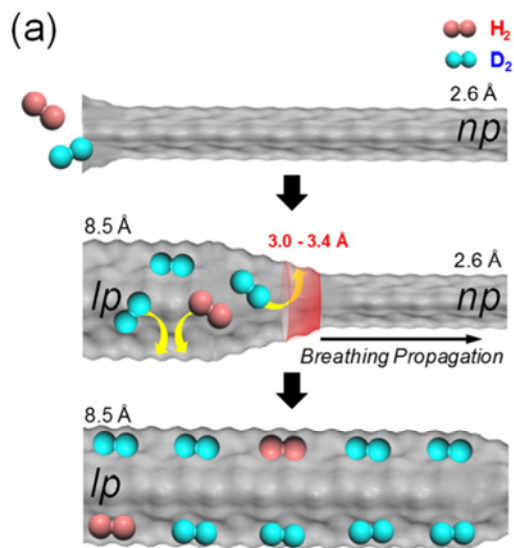
Type: Poster Presentation, Time: THU 11:00~12:30

Selective hydrogen isotope separation via breathing transition in MIL-53(Al)

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Flexibility of metal-organic frameworks (MOFs) is the important feature that is distinguishable from other inorganic porous materials such as zeolite and porous silica. Especially, large changes in the unit cell parameters upon exposure of specific adsorbates showing expansion and contraction, called breathing effect, has attracted the attentions in the field of separation and sorption. In-situ dynamic change of pore aperture triggered by external stimuli, especially gas adsorption, is a very useful phenomenon for the separation of mixtures with similar size and shape (e.g., isotope mixture), requiring precise pore size tuning. Herein, for the first time, we report a strategy for effectively separating hydrogen isotopes utilizing the dynamic pore change during the breathing of flexible MOF, MIL-53(Al). The experiment shows that D_2 over H_2 selectivity is strongly related to the state of pore structure of MIL-53(Al). The highest selectivity (S_{D_2/H_2} 11.6 at 40 K) was obtained via systematically tuning the pore state of MIL-53(Al) by optimizing the exposure temperature and pressure.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-32**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A Chemical Function of Chemically Inert Trichloromethane: Low-Temperature Activation of Open Metal Sites in MOFs

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Open metal site (OMS), coordinatively unsaturated site on metal node in metal-organic frameworks (MOFs), has often shown considerable significance in its role for applications such as gas storage, molecular separation, and ionic and electronic conductions. Thus, the activation of MOFs, the removal of precoordinated solvent molecules (typically used in during the synthesis) at the OMSs, has been thought as an important prerequisite step that must be performed prior to use of the MOFs for the applications. So far, thermal activation that is performed by applying heat and vacuum (hereafter TA) has been considered as a unique method to remove the precoordinating solvent molecules. However, given that high temperature (e.g., >150 °C) has often led to structural damage or complete collapse of MOFs, a low-temperature process for safe activation has been demanded. In this poster, we present a new activation method, “chemical activation”, which is performed at room temperature. More precisely, the chemical activation process is achieved just by soaking MOF samples in trichloromethane (TCM) for several minutes. Using Raman spectroscopic analysis, we provide a plausible mechanism for the activation function of TCM. The efficiency of activation function of TCM is similar to that of TCM-analogous dichloromethane (DCM) at room temperature. However, the efficiency of TCM is substantially enhanced when it applies slightly higher temperature.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-33**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation and Characterizations of High Surface Few Layer Graphitic Mesoporous Carbon Materials

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High surface few-layer graphitic mesoporous carbon materials were prepared from the hard templating method without using porous silica hard template. Crystalline mesoporous ZnO/Zn(OH)₂ spheres with adequate surface area are used as an acid-labile hard template for carbon materials. Furfuryl alcohol (F) or phloroglucinol (P) were employed as the carbon precursors. In the case of N-doped carbon material, melamine was employed as the nitrogen-dopant source. The basic surfaces of ZnO/Zn(OH)₂ are ideal for the polymerization of carbon precursors. After carbonization at 800 °C under N₂ flow followed by an acid etching step, pure carbon materials were fabricated. XPS analysis showed that phloroglucinol gave rise to higher oxygen content in carbon material than furfuryl alcohol. These carbon materials are composed of well-interconnected few layer graphitic structures as revealed by HR-TEM and Raman spectroscopy. Gas sorption analysis displays the surface areas are in the range of 1016 and 1060 m² g⁻¹. N-doped carbon material with BET surface area of 1363 m² g⁻¹ was also successfully prepared from phloroglucinol and melamine. Hydrogen and carbon dioxide uptake abilities were investigated at 77 K and 196 K, respectively. The N-doped carbon material revealed the highest uptake of H₂ (1.69 wt%) and CO₂ (367.4 cm³ g⁻¹). They also presented high CO₂ adsorption enthalpy values. These carbon-based materials yield high capacitances up to 181.3 F g⁻¹. The N-doped carbon material exhibited capacitance retention of 102.7 % after 2000 cycles. Hence, they can be used as supercapacitors with high stability.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-34**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Anisotropic Proton Conduction in a Channel-Type Metal-Organic Framework MOF-74

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The porosity of metal-organic frameworks (MOFs) has demonstrated its potential, especially, in electrochemical applications such as proton conduction. However, the demonstration of high proton conductivity has been limited only to several MOFs, which possess (i) abundant proton sources in pore and/or framework, (ii) large pores to enable to contain sufficient amount of proton-transporting medium, and importantly (iii) high framework stability against water or acid. Among MOFs that can satisfy the aforementioned factors to attain high proton conductivity are MOF-74 and UiO-66. In this poster, we present the anisotropic proton conductivity of robust Co-MOF-74 which contains large 1-dimensional channels along c-axis. More precisely, the MOF-74 shows high anisotropy in proton conductivities that are measured along two different directions: parallel and perpendicular to the c-axis. For example, while the conductivity perpendicular to the c-axis under neutral conditions was approximately 10^{-5} S cm⁻¹, the conductivity parallel to the c-axis exhibited two-order higher value than that of the perpendicular conductivity. Further, we demonstrate that the anisotropic ratios of conductivities are independent on the type of solvent coordinating at Co²⁺ node.

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Code: **INOR.P-35**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Electrochemical Hydrogen Production with New Cyclopentadienyl Rhodium(III) Complexes

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Two new molecular rhodium(III) catalysts were investigated in the electrocatalytic activity for a hydrogen evolution system in the presence of a proton source using glassy carbon electrodes in acetonitrile and water. Rhodium complexes supported by pbi and pbt ligands, i.e., [Cp^{*}Rh(pbt)Cl](PF₆) (1) and [Cp^{*}Rh(pbi)Cl] (2) (where Cp^{*} is pentamethylcyclopentadienyl, pbt is 2-(2'-pyridyl)benzothiazole, and pbi is 2-(2'-pyridyl)benzimidazole), were observed to electrocatalytically evolve H₂ at potential of -0.90 V vs Ag/AgCl in CH₃CN and CH₃CN/H₂O. Cyclic voltammetry of 1 and 2 in the presence of acid revealed redox waves consistent with the Rh(III)/Rh(I) couple. Bulk electrolysis were used to confirm the catalytic nature of the process for complexes 1 and 2, with turnover numbers in excess of 100 and essentially quantitative faradaic yields for H₂ production. The potentials at which these Rh complexes catalyzed H₂ evolution were close to the thermodynamic potentials for the production of H₂ from protons in CH₃CN and CH₃CN/H₂O, with the small overpotential being 50 mV for 1 as determined by electrochemistry. The complex 1 with more positive Rh(III/I) redox potentials exhibited higher activity for H₂ production.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-36**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Diiridium (III) Complexes as Emission Probes for G-quadruplex DNA and Cell Imaging

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DNA G-quadruplex is a four stranded structure, derived from a guanine (G) rich DNA sequence. Though G-rich sequences have been demonstrated to form G-quadruplex structure in vitro, the existence of G-quadruplex structure in vivo is still controversial. Thus detecting G-quadruplex structure has great significance for cell proliferation, cancer research and drug development. Also, imaging of small organelles in the cell such as ER is very important, in understanding the structure and function of these organelles. Herein, two new dinuclear iridium (Ir) complexes bridged by a conjugate aromatic tppz ligand, were prepared. The DNA binding properties of both complexes were studied using single, double stranded and G-quadruplex DNA. Interestingly, the Ir complex demonstrated selectivity for G-quadruplex DNA over other control DNA which was observed by an enhancement in the phosphorescent spectra of the complex. In order to understand their possible interaction with lipid-rich organelles in live cells, the phosphorescent properties of both complexes were studied using liposomes which showed an increased in phosphorescent intensity upon the addition of liposomes with the probe showing a greater enhancement. We also confirmed that the Ir complexes could be used as probes in live cells. The probes were intensely stained in HeLa cervical cancer cells. Excitation with 488 nm laser showed red emission localized in the cytosol of cells. Cellular studies showed that the probes were located inside HeLa cells, but neither complex passed through the nuclear membrane. However, the complexes possessed superior photostability, indicating their role as good luminescent agents for imaging and tracking the endoplasmic reticulum (ER) in live cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-37

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solar-Driven Water Oxidation by *p*-Benzoquinone Derivatives with Non-Heme Iron Complexes

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In photosystem II (PSII), solar-driven water oxidation occurs using plastoquinone (PQ) as an oxidant to produce dioxygen (O₂) and plastoquinol (PQH₂). An early claim to achieve solar-driven water oxidation by *p*-benzoquinone with a di- μ -oxo bridged manganese complex to evolve dioxygen was later withdrawn (*Science* **1974**, 184, 375 & *Science* **1974**, 185, 376). Since then, neither the stoichiometry nor the intermediate of photodriven water oxidation by quinones has been well established. We report herein photodriven water oxidation by *p*-benzoquinone derivatives such as 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ) with a non-heme iron(II) complex ([$(\text{N4Py})\text{Fe}^{\text{II}}$]²⁺; N4Py = *N,N*-bis(2-pyridylmethyl)-*N*-bis(2-pyridyl)methylamine) in acetonitrile (MeCN) containing H₂O (0.50 M). Photoirradiation of an MeCN solution of DDQ (0.50 mM) and [$(\text{N4Py})\text{Fe}^{\text{II}}$]²⁺ (0.20 mM) and H₂O (0.50 M) with a Xenon lamp resulted in O₂ evolution (0.25 mM) in 3 h. The formation of DDQH₂ was confirmed by the absorption and ¹H NMR spectra. The mechanism of photocatalytic oxidation of H₂O by DDQ with [$(\text{N4Py})\text{Fe}^{\text{II}}$]²⁺ will be discussed including the role of the oxidized [$(\text{N4Py})\text{Fe}^{\text{IV}}(\text{O})$]²⁺.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-38**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Hollow Mesoporous Silica Capsule with Few Surface Holes: Efficient Immobilization of Enzymes

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Hollow capsular materials with surface holes are attractive for noncovalent encapsulation of native enzymes or proteins for various applications. In this case, hollow capsular materials with few controllable surface holes are ideal for enzyme encapsulation. Once the enzymes are encapsulated into these materials, the enzymes cannot easily leach out from the capsular materials due to the limited number of surface holes. Contrarily, relatively small substrates freely enter through the surface holes and then converted into desired products inside of capsular materials. By this way, effective enzyme immobilization system with high recyclability can be realized. It is not easy to introduce few controllable surface holes for hollow capsular materials. We developed a new method of preparation of hollow mesoporous silica capsule (HMSC) with few controllable surface holes. Nanosized monodisperse polystyrene (PS) beads were coated with mesoporous silica layer by using CTAB and TEOS in basic condition. Calcination of the resulting material produced HMSC with high surface area. Then, thin nonporous silica layer was additionally coated to make the capsular materials completely nonporous. Mild etching of the HMSC with Ca(II) ions in methanolic solution successfully gave HMSC with few surface holes. The final HMSC was simply immersed into aqueous buffer solutions containing proteins or lipase PS for encapsulation of proteins or enzymes. In order to demonstrate the recyclability of encapsulated enzyme, lipase PS-encapsulated HMSC was subject to biocatalytic transesterification of the racemic 1-phenylethanol with isopropenyl acetate for the production of enantiomerically pure 1-phenylethanol. The catalytic reaction could be repeated multiple times without significant loss of activity.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-39**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nanoporous Copper Silicate, SGU-29 for Partial Oxidation of C-H bond

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By using the zeolite-based heterogeneous catalytic system and its selective reactivity, it is possible to design for the desired chemical reaction. Herein, we report the catalytic activity for partial oxidation of cyclohexane of transition metal oxide molecular sieve, SGU-29 containing square plane-oxygenated Cu active site. We found that cyclohexane was effectively partial oxidized to useful chemical form, cyclohexanol and cyclohexanone through SGU-29 zeolite using *tert*-butyl hydrogen peroxide as oxidant. Catalyst activity of SGU-29 can be optimized by varying the amount of chemicals and reaction temperature. And oxidation of cyclohexane reach ~20% yield of cyclohexanol and cyclohexanone under optimized conditions. Consequently, microporous of transition metal oxide molecular sieve, SGU-29 as catalyst has been proved as one of the excellent candidate for partial oxidation of carbon-hydrogen bonds.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-40**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solution Processed Fabrication of Perfected Oriented Lead Selenide Thin Film

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Solution processed fabrication of perfect oriented lead selenide (200) film on the various substrate such as plane glass, transparent conducting glass and plastic substrate has been achieved for the first time. This research aims to explore the impact of the parameters for orientation such as acetate anion quantity effect, crystallization temperature, and chemical composition on the solution processed lead selenide thin film. In particular, we found that the presence of acetate anion in the precursor solution strongly affected the degree of orientation. A low glancing angle X-ray Diffraction is used and the pole-figure polar distance is scanned by rotating the sample about the direction of the incident beam. Results confirm perfect (200) orientation of prepared lead selenide films. Furthermore, we investigated effect of orientation on the electrical conductivity and thermoelectric properties.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-41

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Noble Titanium(IV) Complexes containing Chiral Tridentate Ligands for Cycloaddition of CO₂ to Epoxides

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CO₂ utilization had been drawn environmentally and economically much attention for a long time. Despite extensive researches, searching for the industrially useful catalytic system still remained as an important research area. As a new titanium catalytic system, two new titanium complexes containing tridentate chiral Schiff-base Ligand, **L**, prepared from condensation reaction with 2,4-pentadione and (1R,2S)-(-)-1-aminoindanol, were synthesized and characterized by various methods including X-ray crystallography. The ligand **L** acted as a dianionic tridentate ligand and had chiral center at amino indanol group, providing chirality to titanium complexes. These complexes were used in the cycloaddition of CO₂ to propylene oxide; both of complexes provided high selectivity of CPC(cyclic propylene carbonate) (>99%) and showed moderate activities compared with the reported catalyst systems.

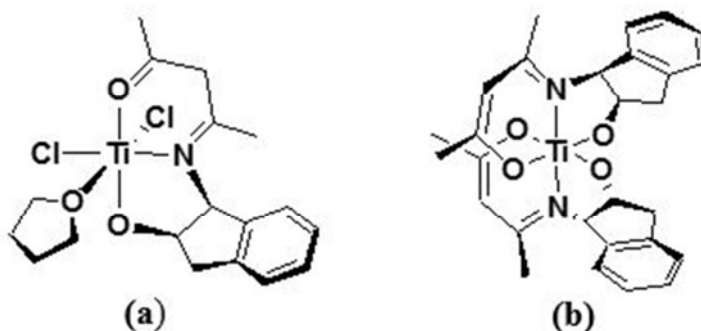


Figure 1. Molecular Structure of Ti Complexes
(a) **TiL(THF)Cl₂** and (b) **TiL₂**

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-42**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The formation of Ruthenium Supramolecules Based on Asymmetric Metalloligands Ligands

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In the supramolecular chemistry, symmetric ligands with ruthenium electron are the most extensively exploited building blocks in coordination-based supramolecular assembly. In contrast, the attempts to utilize asymmetric ligands in the assembly are far less common because the asymmetric system can provide more complicated architectures with larger number of possible products. As a new asymmetric metalloligand system, we designed asymmetric di-ruthenium electron acceptor units possessing electron donating pyridine units. These complexes could have a dual role as a donor as well as an acceptor in the self-assembly to promote additional complexation. Two kinds of asymmetric ligands and corresponding metalloligands were synthesized and characterized by various methods including X-ray crystallography. Simple self-assembly to rectangles and further complexations with additional metal precursor to construct complicated heterobimetallic complex will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-43**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Heterometallic Supramolecular Cage with Homo- or Heteroleptic Aluminum(III) Metalloligands Containing β -diketonate Ligands

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Recent researches in supramolecular chemistry have focused on the heterometallic assembly by means of metalloligand electron donors. β -diketonate ligand possessing pyridyl groups is one of useful and convenient ligands for the formation of octahedral metalloligands. To achieve Al heterometallic supramolecules, we designed aluminum(III) metalloligands containing β -diketonate ligands and used them in the heterometallic supramolecular assembly. The reaction of (tris-{1-(4-pyridyl)acetylacetonato})Al(III)(L1) and diruthenium electron acceptors(A1) resulted in the formation of [2+3] heterometallic trigonal bipyramidal cage. and the other aluminum complex (di(4-pyridyl)-1,3-propanedionato)2(acetylacetonato)Al(III)(L3) and cis-platinumCl2(PEt3)2 electron acceptor(A2) were reacted to produce [4+8] heterometallic tetragonal cage.

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Code: **INOR.P-44**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Cobalt(III) Complex Containing Tetradentate Schiffbase with Pyridoxal for CO₂ Copolymerization

Saem Hwang, Ji Yeon Ryu, Junseong Lee*

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Abstract: In recent years, there have been reports that many cobalt complexes are used by catalyst in different areas. The complexes were often used in CO₂ copolymerization. General cobalt complexes used by catalyst in CO₂ reaction contain salen(N,N'-bis(salicylidene)ethylenediamine)ligand. In this study, the novel cobalt complex containing salen ligand with pyridine was synthesized for developing new cobalt complex system. A new cobalt complex, Co(pyr2en)OAc, was synthesized by the reaction of pyr2en ligands (pyr2en = (N,N'-bis(pyridoxylideneiminato)ethylene)) with Co(OAc)₂. The complex was characterized by various spectroscopic methods such as infrared spectroscopy, HR-MS, single crystal X-ray crystallography. 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 complex was used in the cycloaddition reaction of CO₂ to propylene oxide and the detailed study will be presented.

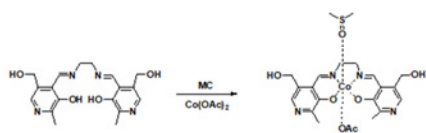


Figure 1: Synthesis of Co(III) complex



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-45**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ruthenium Heterometallic Coordination Cages with High Symmetric Teterapyridyl Metalloligands

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The six coordination cages A_4D_2 or A_6D_3 (A = acceptor, D = donor) were self-assembled from C_4 -symmetric tetrapyridyl metalloligands containing Fe or Co and three different arene-ruthenium donors. All complexes were easily crystallized through slow diffusion in diethyl ether at room temperature, making possible the detailed analysis of the geometry of these cages by X-ray crystallographic study. It was found that flexibility of the acceptor unit highly influences the molecular geometry of these supramolecular architectures, giving rise to A_4D_2 tetragonal prism, A_4D_2 molecular tweezer or A_6D_3 triple-decker complexes. The solution state study elucidated by 1H NMR spectra and ESI-mass spectroscopy was in good accordance with the solid structures, showing that the constructions in the solid state were also maintained in solution state.

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Code: **INOR.P-46**

Area: Inorganic Chemistry

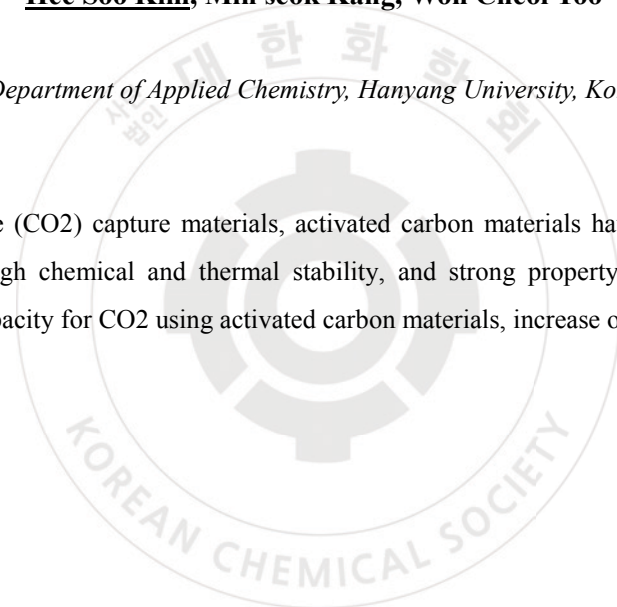
Type: Poster Presentation, Time: THU 11:00~12:30

Highly N-doped Nanoporous Carbon Spheres Derived from Melanin-like Polymer and Biopolymer for CO₂ absorbents and Oxygen Reduction Reaction (ORR) catalysts

Hee Soo Kim, Min seok Kang, Won Cheol Yoo*

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Among carbon dioxide (CO₂) capture materials, activated carbon materials have been of great interest owing to low cost, high chemical and thermal stability, and strong property to humidity. Trying to increase adsorption capacity for CO₂ using activated carbon materials, increase of ultramicropore (



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Code: INOR.P-47

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

New Ni(II), Zn(II) and Co(II) Heptameric Systems from dialdehyde

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We report the three polymetallic heptameric complexes $[\text{Ni}_7\text{L}_6(\mu^3\text{-OH})_6](\text{ClO}_4)_2$ (1), $[\text{Zn}_7\text{L}_6(\mu^3\text{-OH})_6](\text{ClO}_4)_2$ (2) and $[\text{Co}_7\text{L}_6(\mu^3\text{-OH})_6](\text{ClO}_4)_2$ (3), where L=4-tert-Butyl-2,6-diformylphenol. These heptametallic complexes are characterised by IR, NMR (for 2), EA, ESI-MS and X-ray single crystal diffraction. Due to usefulness in gas storage, catalysis, anion sensing recognition and drug delivery superamolecules are of highest interest these days. By the right choice of ligand polymetallic superamolecules can be synthesised which find their application as single molecular magnetic (SMM). By treatment of dialdehyde with metal perchlorate salts of Ni, Zn and Co in the presence of strong base NaOH at temperature 50° C using methanol as solvent and stirring it for 3h, rare heptametallic superamolecules are obtained. The synthesis of these disc shaped heptameric complexes highly depends on the factors including ligand to metal ratios, temperature and the types of base used. These complexes are only obtained in the presence of strong base like sodium hydroxide. To validate the synthetic approach, we used weak base such triethylamine which didn't result in the formation of heptamer system. Due to the unidirectional coordination sites of the ligand the arrangement of metal atoms and the ligand is very sparse. The X-ray structural analysis revealed that cores of these crystals are hexagonal shape of MII ions which surround the central metal ion bridged by $\mu^3\text{-OH}$. The peripheral metal atoms are surrounded by six ligand molecules.

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Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Investigation of geometric and electronic structure of high-valent cobalt complex

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High-valent metal-oxo species are suggested to mediate several important oxidation reaction; C-H bond activation and water oxidation, for instance. Since the transition metal-oxo complexes have a short life time, spectroscopic analysis is thus difficult. Despite of the difficulty in preparing for short-lived metal-oxo species, the identification of the geometric and electronic structures of the species is crucial due to its importance in elucidating the catalytic mechanism. Recently, some studies have found that high-valent cobalt-oxo intermediates are synthesized and successfully captured. In this poster, we will present EPR spectroscopic result of a high-valent cobalt-oxo intermediate. Multi-frequency (9/34/94 GHz) continuous wave (CW) and electron spin echo (ESE) EPR on the cobalt complex were performed and Q-band (34 GHz) electron nuclear double resonance (ENDOR), electron spin echo envelope modulation (ESEEM) and X-band hyperfine sub-level correlation (HYSCORE) experiments were conducted to investigate the electronic structure of the cobalt-oxo intermediate. In addition, Q-band ¹H ENDOR, ¹⁴N ESEEM and X-band ¹⁴N HYSCORE measurements were performed to explore the more detailed geometry of the cobalt complex. This study supports the powerful spectroscopic evidence of the electronic structure of Co^{IV}(O) species.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-49**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Structural and kinetic studies of MMOR ; An EPR Study

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Methane monooxygenase (MMO) is able to turn inert methane into methanol. Therefore, it is gaining significant attention due to its crucial role in the global carbon cycle and to hinder the greenhouse effect by removing methane from the atmosphere. Moreover, the product of MMO's methane oxidation reaction, methanol, is also able to use alternative energy. The soluble form of MMO has three components; (I) Hydroxylase (MMOH), (II) Reductase (MMOR), and (III) β -unit (MMOB). MMOR consists of flavin adenine dinucleotide (FAD) and $[2Fe-2S]^{2+}$ (III,III). It is known that MMOR is involved in electron transfer to MMOH. However, the role of MMOR is not clarified yet. To elucidate the electron transfer pathway of MMOR, we probed the structure and kinetics of electron transfer of MMOR by CW-EPR, pulsed EPR spectroscopy. In addition, we have investigated the effect of MMOB on MMOR in terms of structure and kinetics. To study EPR-silent MMOR at the resting state, we have performed chemical reduction to make it EPR-visible. In addition to confirm the results of chemical reduction experiments, we have carried out cryo-reduction experiments as well. Thus, EPR studies coupled with cryo-reduction and annealing techniques, will provide an essential clue to comprehend the unknown electron transfer pathway of MMOR.

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Code: **INOR.P-50**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Pulse EPR Study of Cu-A β -Inhibitor Ternary Complex; Insight into Working Mechanism of Inhibitor on Cu-A β

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Alzheimer's disease (AD) is a chronic neurodegenerative disease and AD has come to cause serious problems for both individuals and society. Interestingly, high concentration of copper ion has been found in the brain of Alzheimer's patient; it has been proposed that copper ions affect aggregation of the amyloid beta peptide (A β). Recent studies on several inhibitors for Cu-A β aggregates suggest that the inhibitors are able to target and disassemble Cu-A β aggregation. Thus, clarification of the structural information of inhibitors in Cu-A β system is required. In this presentation, we prepared two types of small molecules as inhibitors. To illustrate the structure of ternary complexes of Cu-A β -inhibitor and further elucidate the inhibition mechanism, multi-technique Electron Paramagnetic Resonance (EPR) studies were conducted: 9 GHz Continuous Wave-EPR, 34 GHz pulse Electron Nuclear Double Resonance (ENDOR), and 9 GHz pulse Electron Spin Echo Envelope Modulation (ESEEM). Herein, we will present the structural information of Cu-A β -inhibitor ternary complexes. Our recent results may provide a designing rule of inhibitor molecules for Cu-A β aggregates.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-51**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Flexible Metal-Organic Framework (MOF) Papers Made from MOF Growth on Filter Paper and Their Selective Dye Capture Ability

Jeehyun Park, Moonhyun Oh *

Department of Chemistry, Yonsei University, Korea

The conjugation of metal-organic frameworks (MOFs) with other materials is a brilliant strategy for the production of innovative materials having a desired property and so an appropriate applicability. In particular, the integration of MOFs with a flexible paper is expected to form valuable materials for the separation technology. Among the various MOF materials, zeolitic imidazolate frameworks (ZIFs) are particularly interesting because they are stable in water and can therefore be applied for operations in aqueous media. Therefore, the integration of water stable ZIF materials with a flexible filter paper would provide a rapid and convenient route for the generation of flexible MOF materials that could be useful for the separation of organic dyes in water. Herein, a facile method for the generation of MOF-based papers has been reported which involves the conjugation of carboxymethylated filter paper (CMFP) and ZIF nanoparticles. A compact and uniform growth of ZIF nanoparticles on the cellulose surface of CMFP results in the formation of the flexible CMFP/ZIFs. As a result of the compact coating, the resulting CMFP/ZIFs display an effective capture ability for organic dyes when their solutions are subjected to a simple filtration. In addition, the CMFP/ZIF materials can be reused for the dye separation after a simple washing process.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-52**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation and Electrochemical Properties of 1,1-Diethyl(or Dihexyl)-3,4-diphenyl-2,5-disubstitutedsiloles

JiYoung Park, Young Tae Park*

Department of Chemistry, Keimyung University, Korea

Silacyclopenta-2,4-dienes called as siloles are a series of five-membered silacyclic dienes with π -electron system containing low-lying lowest unoccupied molecular orbital(LUMO) level. For the synthesis of 1,1-diethyl(or 1,1-dihexyl)-3,4-diphenyl-2,5-disubstitutedsiloles, diethyl or dihexylbis(phenylethynyl)silanes as precursors were prepared by reactions of dichlorodiethylsilane or dichlorodihexylsilane with phenylacetylene treated with *n*-butyllithium in situ, in the first step. In the second step, several derivatives of 1,1-diethyl or 1,1-dihexyl-3,4-diphenyl-2,5-disubstitutedsiloles were synthesized by the intramolecular reductive cyclizations of diethyl or dihexylbis(phenylethynyl)silanes with treatments of lithium naphthalenide and followed by reactions with anhydrous $ZnCl_2$ and N-bromosuccinimide, trimethylchlorosilane in situ, and coupling reaction with ethynyltrimethylsilane, respectively. The crude products were purified by recrystallization in hexane. The obtained silole derivatives are soluble in usual organic solvents such as THF and $CHCl_3$. We have studied the electronic properties of the polymeric silolene materials containing with disubstitutedsilylene by using UV-vis absorption, excitation and fluorescence emission spectroscopic methods. The prepared materials here were characterized by 1H , ^{13}C NMR, and FT-IR spectroscopies along with TGA. We studied the electronic properties such as UV-vis absorption, excitation, and fluorescence emission spectra of the obtained siloles. We examined electrochemical properties of the prepared 3,4-diphenyl-2,5-disubstitutedsiloles, 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).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-53**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Optical Properties of Salen-Indium/Triarylborane Triads

Sang Woo Kwak, Kang Mun Lee¹, Min Kim, Youngjo Kim, Yongseog Chung^{*}, Myung Hwan Park^{2,*}

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Salen-In(CH₃) complexes bearing dimesitylborane units (1) and dimesityl(phenyl)borane (2) at C5 positions of salen moieties were prepared and fully characterized. The major absorption bands of 1 and 2 are shown in the region centered at ca. 347 nm for 1 and ca. 374 nm for 2 and the intense emission spectra for these compounds are observed in the sky blue ($\lambda_{em} = 491$ nm for 1) and bluish-green (498 nm for 2) region, respectively. The solvatochromism effects in various organic solvents and theoretical calculation results strongly suggest that these absorption and emission spectra are mainly involved to intramolecular charge transfer (ICT) transitions between salen ligand moieties to triarylborane units. UV-vis and PL titration experiments with the addition of fluoride anions demonstrate ratiometrically quenching patterns in both absorption and emission spectra, indicating that the fluoride binding to boron centers interrupt such the ICT transitions in each compound. Interestingly, both compounds also show gradually red-shifted response upon the addition of fluoride anions in each emission spectrum, resulting in dramatic color-change to yellow. Theoretical calculation results on the S1 states imply that these red-shifted 'color-change' properties arise from the elevation of HOMO levels due to the fluoride anion binding.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-54**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Structural variations in new molybdenum oxyfluorides

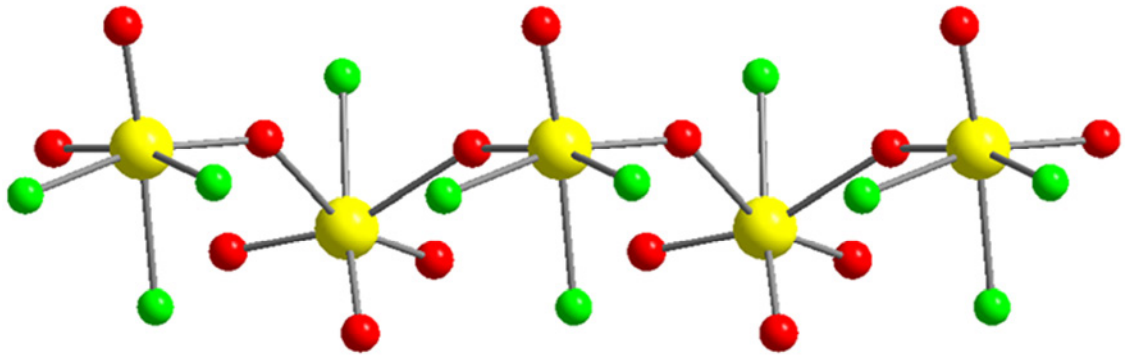
Hongil Jo, Jung Joo Kim¹, Lee HyeEun¹, Kang Min Ok^{*}

Department of Chemistry, Chung-Ang University, Korea

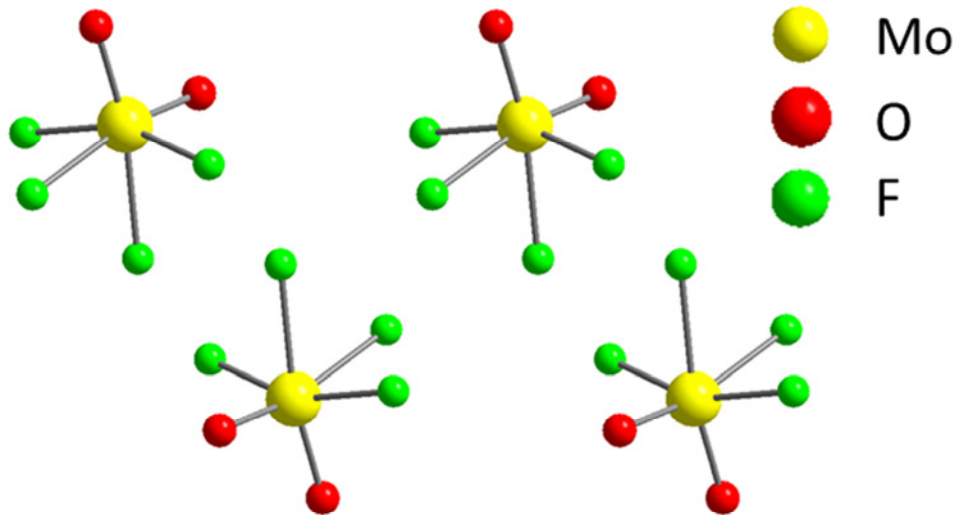
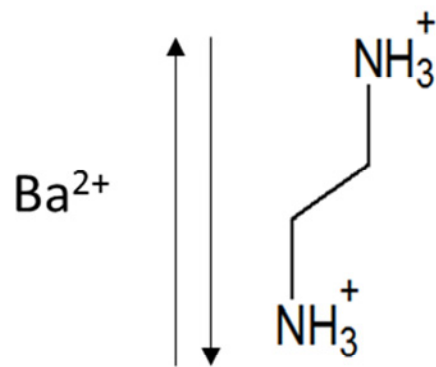
¹*Chung-Ang University, Korea*

Molybdenum oxyfluorides have been studied for O/F ordering, linkage of octahedral $\text{MoO}_x\text{F}_{6-x}$, and second-order Jahn-Teller distortions. Thus far, most of the studies have been conducted using monovalent cations such as alkali metal and organic ammonium cations. In this study, we used divalent cations such as Ba^{2+} and organic diammonium cations and successfully synthesized $[\text{A}]^{2+}[\text{MoO}_x\text{F}_y]^{2-}$ through hydrothermal reactions.

BaMoO_3F_2 crystallizes in the monoclinic space group, $P2_1/n$ and shows one-dimensional $[\text{Mo}_2\text{O}_6\text{F}_4]_\infty$ chains that are surrounded by Ba^{2+} . $[\text{enH}_2]\text{MoO}_2\text{F}_4$ crystallizes in the triclinic space group, $P-1$ (en = ethylenediamine, $\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2$) and reveals a molecular structure consisting of $[\text{enH}_2]^{2+}$ and distorted $[\text{MoO}_2\text{F}_4]^{2-}$ octahedral. Various synthetic efforts indicate that large divalent cations stabilize the structures of molybdenum oxyfluorides. In this presentation, we will show how MoO_xF_y octahedra will vary by changing divalent cations. Detailed crystal structures, spectroscopic characterization, and thermal analyses for the compounds will be presented.



Corner sharing



Isolated

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-55**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

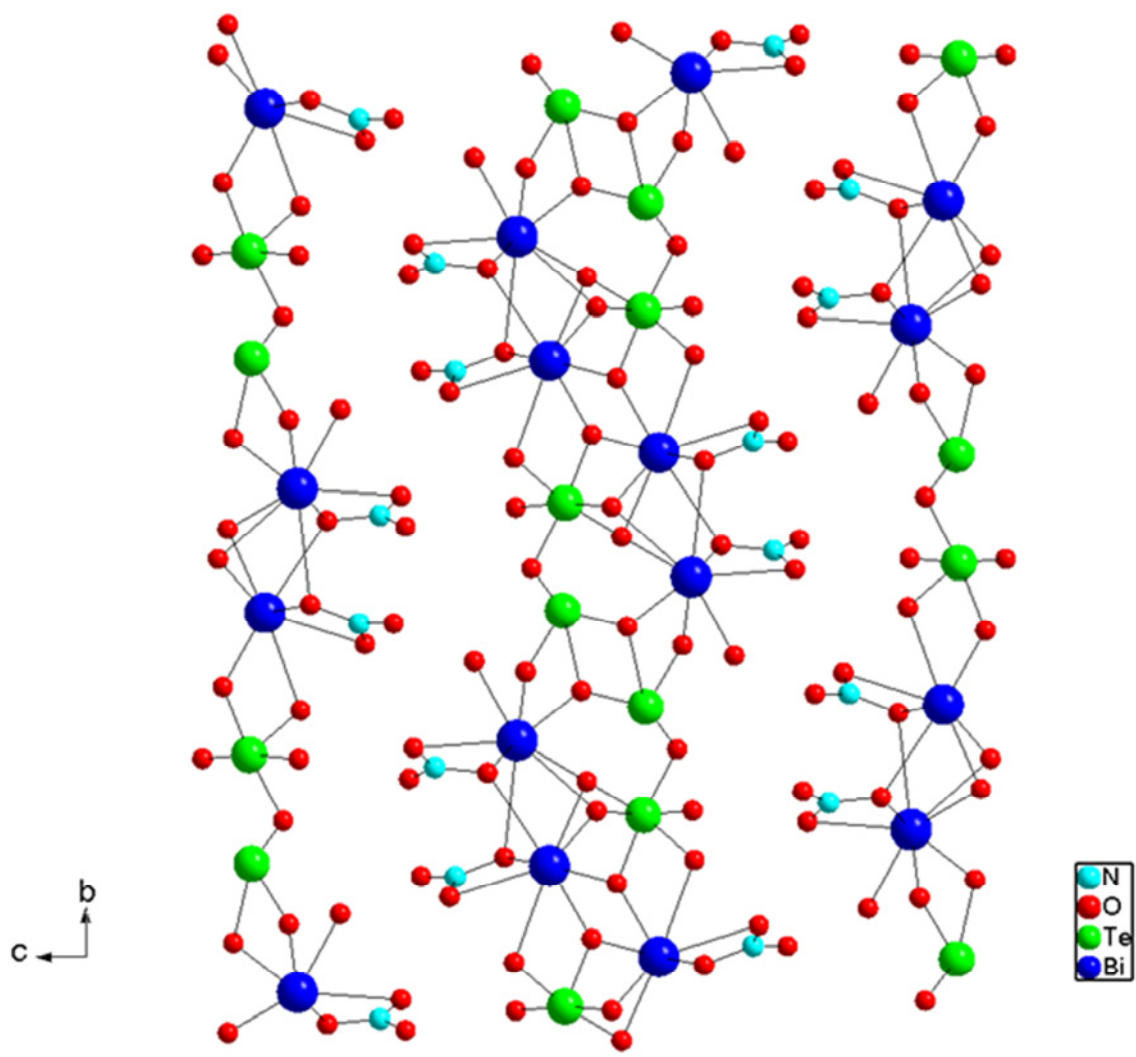
Synthesis and nonlinear optical properties of noncentrosymmetric $\text{Bi}_2\text{Te}^{4+}\text{Te}^{6+}\text{O}_6(\text{NO}_3)_2(\text{H}_2\text{O})(\text{OH})_2$

So Yon Lee, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

Noncentrosymmetric (NCS) materials may reveal properties such as pyroelectricity, piezoelectricity, ferroelectricity, and nonlinear properties that can be used in various industrial fields. NCS materials cannot be obtained if there is an inversion center in a unit cell. Therefore, bismuth and tellurium, which both have stereochemically active lone pairs and NO_3^- with a π - conjugation effect were used.

$\text{Bi}_2\text{Te}^{4+}\text{Te}^{6+}\text{O}_6(\text{NO}_3)_2(\text{H}_2\text{O})(\text{OH})_2$ has been synthesized by a hydrothermal reaction. The compound crystallizes in the NCS nonpolar space group, $P2_12_12_1$. This product exhibits a layered structure with a water molecule bonded between the layers. The framework consists of BiO_9 and BiO_{10} polyhedra and NO_3 . Tellurium shows two coordination environments, i.e., Te^{4+} as a see-saw form and Te^{6+} as an octahedral form. This material reveals a second harmonic generation efficiency of 20 times that of α - SiO_2 .



KOREAN CHEMICAL SOCIETY

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Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-56

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

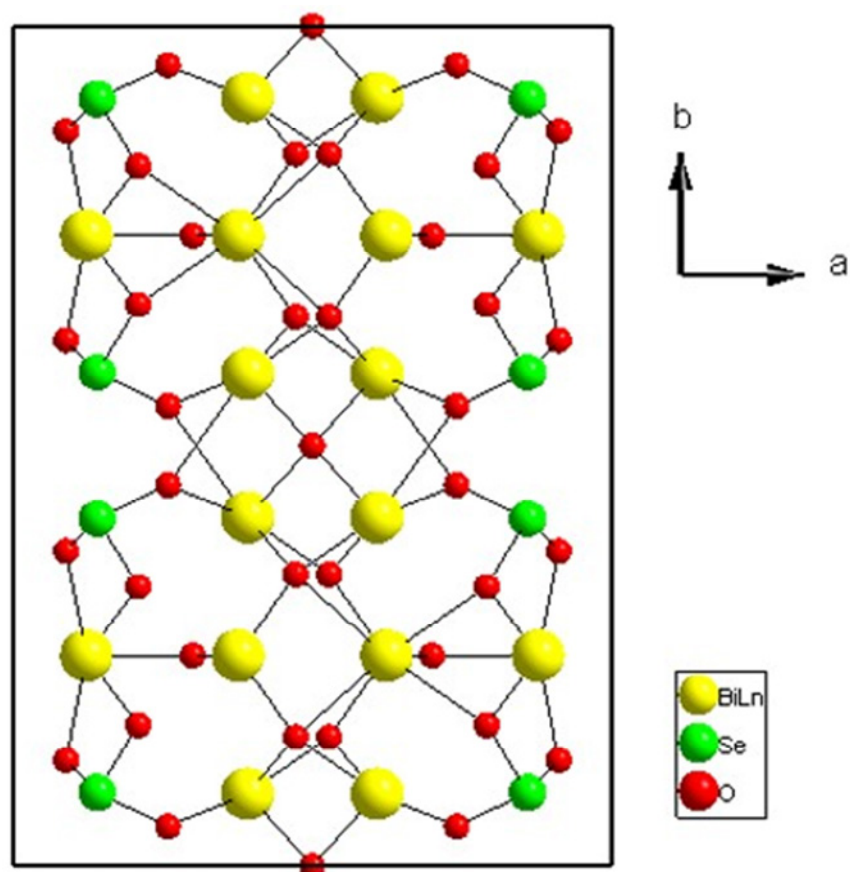
Synthesis and second-harmonic generation properties of noncentrosymmetric bismuth selenite solid solutions, $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$ (Ln = La, Eu; $x = 0-0.3$)

Haixin Qi, HYERIN SONG¹, Kang Min Ok^{*}

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¹*Chung-Ang University, Korea*

A series of La^{3+} or Eu^{3+} -doped noncentrosymmetric (NCS) bismuth selenite solid solutions, $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$ ($x = 0-0.3$), have been successfully synthesized via standard solid-state reactions with Bi_2O_3 , La_2O_3 (or Eu_2O_3), and SeO_2 as starting materials. Crystal structures and phase purities of the resultant materials were thoroughly characterized by powder X-ray diffraction using the Rietveld method. The results clearly revealed that the reported materials crystallize in the orthorhombic space group, $Abm2$ (No. 39), and exhibit pseudo-three-dimensional frameworks that are composed of BiO_3 , BiO_5 and SeO_3 polyhedra. Detailed diffraction studies show that the cell volume of $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$ decreases with an increasing amount of Ln^{3+} on the Bi^{3+} sites. However, no ordering between Ln^{3+} and Bi^{3+} was observed in the $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$ solid solutions. Powder second-harmonic generation (SHG) measurements, using 1064 nm radiation, reveal that SHG efficiencies of $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$ solid solutions continuously decrease as more Ln^{3+} cations are added to the sites of polarizable Bi^{3+} cations. The reduction in SHG for Ln^{3+} -doped materials is consistent with the lack of net moment originating from polyhedra with a polarizable Bi^{3+} cation.



Ball and stick model of $\text{Bi}_{2-x}\text{Ln}_x\text{SeO}_5$



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-57**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Thin Coating of Microporous Organic Network Enhances Bending Sustainability of Ni on the PET Textile for Flexible Lithium Ion Batteries

Chang Wan Kang, Jaewon Choi, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

This presentation shows interesting properties of microporous organic network (MON) materials in the critical issue for flexible electrical devices. MONs are a new class of functional materials. Thus, they have much potential to show unexplored properties. The MON materials are comparable to covalent organic framework (COF) and non-porous polymers. The main properties of MON are their microporosities and non-crystalline structure. We discovered that the amorphous structure and microporosity of MONs are beneficial in the realization of sustainable and flexible Ni electrode. These days, the realization of flexible batteries is becoming important. Especially, flexible electrodes are critical. Although the fundamental studies and new approaches are important for the flexible electrodes, this field is at an early stage. Ni was directly deposited on polyethylene terephthalate fibers (PET-Fs). The PET-F@Ni sharply lost the conductivity in the repeated bending. We found that the Ni layers were broken and detached from the PET fibers during the repeated bending tests. In contrast, PET-F fibers were homogeneously coated with a thin MON coating. Then, Ni was deposited on the MON of PET-F@MON fibers. The PET-F@MON@Ni showed excellent retention of electrochemical performance against the repeated bending. According to the SEM analysis, Ni layers were neither broken and nor detached from PET-F@MON after the repeated bending tests. Through the model studies, we found that MON layers play roles as the structural buffers (such as lubricant materials) due to their amorphous characteristic and the resulting structural flexibility and as the binders to attach the Ni to PET platforms due to the high surface areas and microporosities.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-58**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nanoseeds based on SiO₂@sulfonated microporous organic polymer for antifouling terpolymerization of CO, ethylene, and propylene

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Recently, the catalytic synthesis of useful materials using C1 feedstocks is gaining green credentials because of environmental concerns. As a representative issue, the catalytic synthesis of polyketone-based plastic materials has attracted the increased attention of scientists. The homogeneous Pd catalysis for polyketones often suffers from a reactor fouling and the resultant poor quality polymers with high PDI values. To obtain high quality polyketone terpolymers, the catalytic polymerization process should be appropriately controlled. In this regard, the seeded catalysis is promising. However, there have been no sufficient studies on the seeded catalysis for polyketone terpolymers. This presentation shows that the efficient seed materials with SiO₂@sulfonated microporous organic polymer (MOP) structure resulted in good quality polyketone terpolymers with 0~4.5w% insertion of propylene. The size of nanoseeds was controlled from 750 nm to 190 nm. The size of nanoseeds was critical to obtain the granular terpolymers. Moreover, the SiO₂-190@S-MOP system showed a good activity of 17.2 Kg polymer/g-Pd, comparable to the homogeneous system with 19.6 Kg polymer/g-Pd. While the homogeneous system showed a severe reactor fouling and a wide distribution of polymer chains, the SiO₂-190@S-MOP system resulted in the narrow chain distribution without a reactor fouling. We believe that more various nanoseeded catalytic polymerization can be developed using new nanoseed materials adopting the MOP chemistry.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-59

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis, Structural Characterization of 5-Coordinate Copper(II) Complexes Containing *N,N',X*-Iminomethylpyridine Derivatives

JOUNG HEO, Hyosun Lee *

Department of Chemistry, Kyungpook National University, Korea

We have synthesized and characterized a series of new copper(II) complexes, namely $[L_nCuCl_2]$ with ligands $[L_n]$ ($L_n = L_A - L_D$), where ($L_A = (E)$ -2-(piperidin-1-yl)- N -(pyridin-2-ylmethylene)ethanamine), ($L_B = (E)$ -2-methoxy- N -(pyridin-2-ylmethylene)ethanamine), ($L_C = (E)$ -3-methoxy- N -(pyridin-2-ylmethylene)propan-1-amine) and ($L_D = (E)$ -3-(methylthio)- N -(pyridin-2-ylmethylene)propan-1-amine). New Cu(II) complexes are characterized by spectroscopic methods such as IR, elemental analyzer and X-ray single crystal diffraction.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-60**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Copper(II) Complexes with *N'*-substituted *N,N',N*-bis((1H-pyrazol-1-yl)methyl)amine Ligands

hyungwoo cho, Hyosun Lee^{*}

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of Cu(II) complexes with ligands L_n ($L_n = L_A - L_C$) where $L_A = N,N$ -bis((1H-pyrazol-1-yl)methyl)-2,4,6-trimethylbenzenamine, $L_B = N,N$ -bis((1H-pyrazol-1-yl)methyl)-4-methoxybenzenamine, $L_C = N,N$ -bis((1H-pyrazol-1-yl)methyl)-4-fluorobenzenamine. All complexes were characterized by various spectroscopic methods. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were investigated at 60 °C.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-61**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Cobalt(II) Complexes Containing Tridentate *N,N',X*-Iminomethylpyridines: Synthesis, structural characterization and application to polymerization of methyl methacrylate

jae gyeong Lee, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of cobalt(II) complexes by the reaction of $[\text{CoCl}_2]$ with tridentate ligands $[\text{L}_n]$ ($\text{L}_n = \text{L}_A - \text{L}_C$), in which $\text{L}_A = (E)\text{-}N\text{-}(2\text{-morpholinoethyl})\text{-}1\text{-}(\text{pyridin-}2\text{-yl})\text{methanimine}$, $\text{L}_B = (E)\text{-}N\text{-}(2\text{-methoxyphenyl})\text{-}1\text{-}(\text{pyridin-}2\text{-yl})\text{methanimine}$ and $\text{L}_C = (E)\text{-}N\text{-}(2\text{-methylthio})\text{phenyl})\text{-}1\text{-}(\text{pyridin-}2\text{-yl})\text{methanimine}$, respectively. New cobalt(II) complexes were characterized by various spectroscopic methods. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) were also investigated.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-62**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Palladium(II) and Zinc(II) Complexes Containing 4-Methoxy-*N*-((pyridin-2-yl)methylene)benzenamine Derivatives

Suhyun Park, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized and structurally characterized a series of new palladium(II) and zinc(II) complexes, namely $[L_nPdCl_2]$ and $[L_nZnCl_2]$, respectively supported by ligands L_n ($L_n = L_A - L_C$), where $L_A = 4$ -methoxy-*N*-((pyridin-2-yl)methylene)benzenamine, $L_B = 4$ -methoxy-*N*-((pyridin-2-yl)methyl)benzenamine, $L_C = 4$ -methoxy-*N*-methyl-*N*-((pyridin-2-yl)methyl)benzenamine. Molecular structure of $[L_CPdCl_2]$ exhibited 4-coordinate distorted square planar geometry around palladium metal center. Molecular structure of $[(L_B)_2ZnCl_2]$ exhibited 6-coordinate octahedral geometry around zinc metal center. All complexes were characterized by 1H NMR, ^{13}C NMR, elemental analysis (EA), IR. The catalytic activity of palladium(II) and zinc(II) complexes for methyl methacrylate (MMA) polymerization in the presence of modified methylaluminoxane (MMAO) were investigated: $[L_BPdCl_2]$ (3.80×10^4 g PMMA/mol Pd•h) showed the highest catalytic activity compared to rest of complexes in the current study.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-63**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Copper (II) Complexes Containing *N,N*-bis((1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amines

jaeyoung Seo

Department of Chemistry, Kyungpook National University, Korea

New Cu(II) complexes, namely $[L_nCuX]^+Y^-$ ($L_n = L_A - L_D$; $X = NO_3$; $Y = BPh_4, NO_3, ClO_4$) were synthesized by the reaction of $[Cu(NO_3)_2]$ with the corresponding ligands such as *N,N*-bis((1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amine (L_A) and *N,N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amine (L_B) and *N,N*-bis((1H-pyrazol-1-yl)methyl)-1-(pyridin-2-yl)methanamine (L_C) and *N,N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-1-(pyridin-2-yl)methanamine (L_D), in the presence of $NaBPh_4$ or $NaClO_4$, respectively. Molecular structures of these complexes were characterized by X-ray crystallography. Catalytic property of Cu(II) complexes toward the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) were investigated at 60 °C.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-64**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Isomer Effects on the Terphenyl Backbone Based Benzimidazole Electron Transporting Materials

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¹*Department of Applied Chemistry, Daegu University, Korea*

Electron transport material (ETM) in organic light emitting diodes (OLED) is one of the very important material to achieve highly efficient and stable device performance. Especially, there are critical issues in ETM including triplet energy band gap, electron mobility, and thermal stability for blue phosphorescence OLED (PHOLED). Recently, various types of metal chelates, oxadiazole, quinoline, imine, triazole, triazine, and pyridine containing ETM are reported and high triplet energy ETMs for blue PHOLED are also reported by various research groups. For the highly efficient blue PHOLED, high triplet band gap ETM is required to confine the triplet light emission in emission layer in OLED. At the same time, high electron mobility is also needed. However, to design and synthesis of the high triplet energy with high electron mobility material is challengeable due to the tradeoff relationship between triplet energy and electron mobility. In this research, we have designed and synthesized three different terphenyl backbone (ortho-, meta-, and para-terphenyl) based benzimidazole ETMs to understand structure-properties relationship and we are aiming to suggest the design strategy of the high triplet energy with high electron mobility ETM. The photophysical and electrochemical properties of the three different benzimidazole terphenyl isomers were compared each other. In the photophysical and electrochemical properties, the ortho and para isomers show charge delocalization properties through imidazole and terphenyl moiety in the different pathway, which showing the through space (ortho) and through bond (para) delocalization. Due to the efficient charge delocalization by the through bond pathway, the para isomer results low triplet energy gap, which is not suitable for blue PHOLED. In contrast with the ortho and para isomers, the meta isomer shows charge localization property and results high triplet energy gap. In the DFT/TDDFT calculations, this result is well agreed with experimental data. From these data, we assumed that the meta compound is better for high triplet energy but electron charge is destabilized. In conclusion, the ortho

isomer is suitable for the high triplet energy with high electron mobility properties due to the through space charge delocalization by the through space pathway.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-65**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation of Covalent Triazine Frameworks Tuned by mixed-building block strategy for Advancing the Porosity and Hydrophobicity

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inorganicchemistry, Kookmin University, Korea

¹*Department of Chemistry, Kookmin University, Korea*

²*Department of Bionano Chemistry, Kookmin University, Korea*

Controlling the pore structures of catalytic supports in heterogeneous system is essential for both the facile incorporation of metal single-site catalysts and efficient mass transfer of substrates into the active sites of a catalyst. In this regard, covalent triazine frameworks have been functionalized with the rational design of the monomers, resulting in diversely tuned pore natures such as pore size, volume, and chemical/physical properties such as hydrophobicity. Accordingly, we present the synthesis of novel CTFs using mixed monomers (based on bipyridine and phenyl building block) under ionothermal conditions (ZnCl₂ as Lewis acid catalyst, and at 400 °C). We expect that bipyridine-based monomers work as a binding site for transition metal complex and phenyl-based building blocks play a role for tuning the feature of the pore environment. For verifying the pore characters of mixed-CTFs, Brunauer-Emmett-Teller, Element Analysis, H₂O Isotherms were performed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-66**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Tailoring Nanocrystalline MOFs as Fluorescent Dye Carriers for Bioimaging

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Challenges have been exist to take advantage of dye molecules for reliable and reproducible molecular probe in biomedical applications. In this study, we show how to utilize the dye molecules for bioimaging within protective carriers of nanocrystalline metal-organic frameworks (nMOFs) particles. Specifically, Resorufin and Rhodamine-6G having different molecular size were encapsulated within close-fitting pores of nMOF-801 and nUiO-67 particles, respectively. The resulting nanocrystalline particles have high crystallinity, uniform size, and morphology, as well as preserve enhanced photoluminescence properties with exceptional stabilities in biomedical environment. The samples are further functionalized with targeting agent and successfully working for fluorescence imaging of FL83B (human hepatocyte cell) and HepG2 (human hepatocellular carcinoma) without cytotoxicity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-67**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Microporous and Hollow Cr(III)-F Porphyrin Networks for CO₂ Fixation to Cyclic Carbonate at Room Temperature

MyungHyun Kim, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Chemical CO₂ fixation has attracted great attention of scientists. One of the facile CO₂ fixation methods is the reaction of CO₂ with epoxides to form cyclic carbonates which are important polymer precursors, solvent of electrolytes for secondary batteries, etc. This CO₂ fixation process usually requires high reaction temperatures and pressure despite being an exothermic reaction. Lewis acids including Zn or Cr-compounds can accelerate this reaction and can therefore lower the reaction temperature below 100°C. Furthermore, Heterogeneous catalysts for CO₂ fixations have been developed to allow recycling of Lewis acids. Microporous organic networks (MONs) are a new class of functional materials with high surface areas. The microporosity of MONs enables substrates to diffuse into the materials. Hence, the Lewis acid sites in inner MONs can be utilized in chemical conversions. This presentation shows that the MONs can be engineered to form hollow structures with thin shells (shell thickness < 50 nm) by template methods. Hollow and microporous Cr(III)-F porphyrin networks (H-MCrPN) showed the best catalytic activities in the room temperature CO₂ fixation with epoxides to cyclic carbonates. The excellent performance of H-MCrPN is attributed to its microporosity, the short diffusion pathways for substrates due to the hollow structure, and the efficient Lewis acidic activity of Cr(III)-F moieties.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-68**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Correlation between conductivity changes and structural transformations in Zn coordination complexes depending on relative humidity conditions

Jeonghwa Song, Dongwon Kang, Hangeul LEE, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

We prepared three types of Zn-based coordination systems $[\text{Zn}(\text{H}_2\text{SSA})_2(\text{H}_2\text{O})_2]$ (1), $[\text{Zn}(\text{H}_2\text{O})_6] \cdot 2(\text{H}_2\text{SSA}) \cdot 2(\text{H}_2\text{O})$ (2) and $[\text{Zn}(\text{H}_2\text{O})_6] \cdot 2(\text{H}_2\text{SSA}) \cdot 4(\text{H}_2\text{O})$ (3) using the H_3SSA ligand (H_3SSA =5-sulfosalicylic acid). Compound 1 exhibits structural transformations and considerable changes in proton conduction properties under different relative humidity conditions. To elucidate the structural change process, we characterized each phase using PXRD. Detailed understanding of proton dynamics in the frameworks will be given in the presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-69**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Luminescent Cd-based metal-organic frameworks for Mg²⁺ ion sensing

**Sunhui EOM, Jeong eun KIM, Hangeul LEE, Hwa Young Lee, MINJUNG KANG,
jeonghwa Song, Dongwon Kang, Jong Hyeak Choe, Chang Seop Hong***

Department of Chemistry, Korea University, Korea

We synthesized [Cd₃(TCBPA)₂(H₂O)]₃(DMF)₅(H₂O) (Cd-MOF) via the solvothermal reactions. Cd-MOF was characterized by single crystal X-ray diffraction analysis, thermogravimetric analysis, infrared spectroscopy, and elemental analysis. This Cd-MOF can detect specific metal ion. In particular Cd-MOF showed 'turn-on' sensing for Mg²⁺ ion. To the best of our knowledge, Cd-MOF exhibited the best luminescence enhancement for Mg²⁺ sensing reported so far. Detailed synthetic scheme and specific properties will be presented in the poster.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-70**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Extended porous organic polymer conductor exhibiting the superprotonic conductivity ($>0.1 \text{ S cm}^{-1}$) via a Postsynthetic Method

**Dongwon Kang, jeonghwa Song, Hangeul LEE, Jeong eun KIM, Hwa Young Lee,
MINJUNG KANG, Sunhui EOM, Jong Hyeak Choe, Chang Seop Hong***

Department of Chemistry, Korea University, Korea

As potential solid electrolytes in proton exchange membrane fuel cells (PEMFC), many porous conductors have shown fascinating proton conductivities (up to $\sim 10^{-2} \text{ S cm}^{-1}$). To replace Nafion ($\sim 10^{-1} \text{ S cm}^{-1}$), even higher performance is needed for real applications. In this work, we prepared a biphenyl-based porous framework of 1E as an extended version of a phenyl-based framework in our previous work. The sulfonated material, 1ES, was modified via direct postsynthetic substitution and the conductivity of 1ES reached $1.59 \times 10^{-1} \text{ S cm}^{-1}$ at 80 °C and 90% RH. To the best of our knowledge, this is superior to that observed for any POP conductor reported so far, and even surpasses that of Nafion. Detailed synthetic scheme and several properties will be given in the presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-71**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Metal-Organic Frameworks with MOF-74 Type Extended Structure for Gas Adsorption with Acidic Centers

**Hangeul LEE, Dongwon Kang, jeonghwa Song, Hwa Young Lee, Jeong eun KIM, Sunhui
EOM, MINJUNG KANG, Jong Hyeak Choe, Jong Hyeak Choe***

Department of Chemistry, Korea University, Korea

A series of metal–organic frameworks (MOFs) $M_2(\text{dondc})$ ($M = \text{Mg, Mn, Co, Ni}$; $\text{H}_4\text{dondc} = 1,5\text{-dioxido-2,6-naphthalenedicarboxylic acid}$;) were prepared by microwave reactions. From the synchrotron powder X-ray diffraction, the structures of the samples were formed by incorporating dondc^{4-} anions and M^{2+} cations, leading to the construction of a three-dimensional framework consisting of hexagonal channels running along the c axis. These materials have a high density of open metal sites along hexagonal channels. These results are highly correlated with the CO_2 adsorption enthalpy. And these materials are demonstrated to bind CO reversibly. Detailed results will be given in the presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-72**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Hollowing out MOFs: hierarchical micro- and mesoporous MOFs with tailorable porosity via selective acid etching

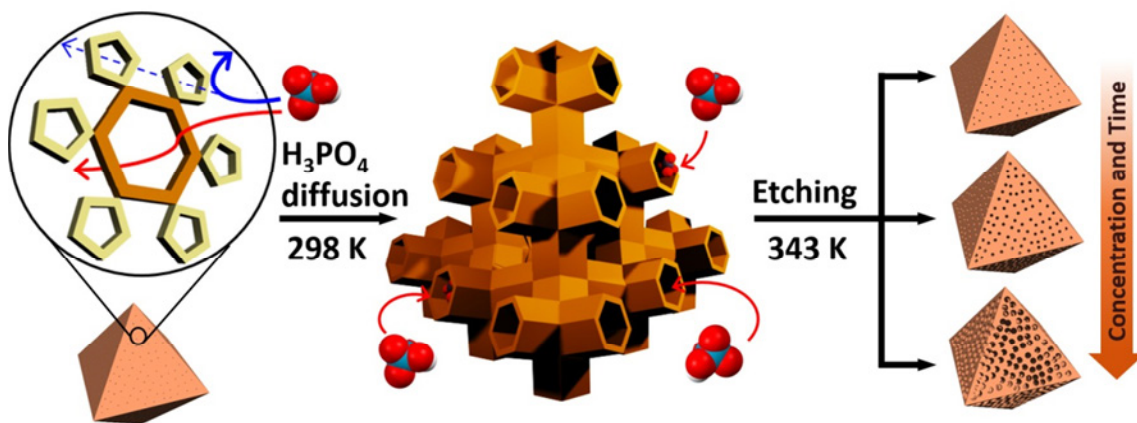
Jaehyoung Koo, In-Chul Hwang¹, Xiujun Yu¹, Kimoon Kim^{2,*}

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*

With increasing interests on metal-organic frameworks (MOFs), post-synthetic modification method receives considerable attention to get more control over the materials, as a pre-synthesized highly porous and desirable framework can be chosen for further modification to fine tune the pore environment without disrupting the framework topology. In 2009, we reported the complete exchange of framework-constituting metal ions from microporous frameworks keeping the original framework topology intact. Extending this work, recently we have demonstrated a partial removal of metal ions of MOFs can generate larger pores with preserving the original microporous framework. As a first example, we presented a post-synthetic transformation from microporous MOF to hierarchical micro- and mesoporous MOF. This unique transformation is achieved by treating microporous MOF POST-66 with water. However, this method is only applicable to MOFs with low water stability and fine-tuning of pore size still needs to be addressed. Here, we report a new novel strategy for the synthesis of water-stable hierarchical porous MOFs by a selective acid etching process (Scheme 1). The process is controlled by the size-selective diffusion of acid molecules through the MOF windows. This method enables the fine-tuning of the porosity of hierarchical MOFs, allowing for the generation of well-defined mesopores with high mesopore volume. Because of the size-selective diffusion of acid molecules, the inherent crystallinity and external morphology of the resulting MOFs are well-maintained after acid treatment. This novel strategy may provide an alternate route towards the synthesis of diverse hierarchical MOFs.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-73**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

One-pot synthesis of stable phenazine radical crystal for new molecular semiconductor

Taeyeon Kwon, Hee Cheul Choi*

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

In this presentation, we will show a simple, rapid synthesis of phenazine radical crystals, potentially applicable as a new molecular semiconductor. The phenazine radical crystals are successfully synthesized under ultraviolet (UV) irradiation in an acidic condition, resulting in rod-shaped black crystals. Although phenazine radicals are known as unstable and sensitive to oxygen, the newly synthesized phenazine radical crystals show high stability at ambient condition. In-situ UV-VIS and electron spin resonance (ESR) spectroscopy were carried out for the resulting crystals, and the results provide the evidence of photoinduced radical formation. Single crystal X-ray analysis revealed a slip-stacking structure of phenazine radical molecules with a strong π - π interaction, which is to the best of our knowledge the first example of stable phenazine cation radical crystals. Electric conductivity of the black crystals showed a linear I-V characteristics (Ohmic contact) along the stacking direction. We believe that our findings would contribute to the development of new stable radical materials and provide an insight into electrically active molecular systems.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-74**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly efficient growth of morphologically well-defined molecular crystals of phenothiazine using drop-drying method in a mixed solvent system

Yurim Ahn, Hee Cheul Choi^{1,*}

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

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

In this presentation, we present a simple, efficient growth of morphologically well-defined phenothiazine crystals by drop-drying its solution composed of mixed solvents. The drop-drying method, which is one of the simplest ways to grow crystals, often fails to grow crystals with well-defined facets in specific morphologies, because it is difficult to control the evaporation of solvents that is necessary for making the solution to reach to supersaturation point, after which nucleation and growth into crystals are proceeded and the morphology of the crystal is also determined. Our strategy to solve this problem is to use a mixture of solvents; a proper combination of volatile and non-volatile solvents would result in a sequential evaporation of each solvent, so the coffee ring effect, which hinders uniform growth of crystals, could be largely suppressed. To prove our concept, we chose phenothiazine as a target solute, because it is a well-known p-type semiconductor but lacks a solution-based method for growing them into morphologically well-defined crystals. The solvent we used is a mixture of non-volatile mesitylene and volatile alcohols such as methanol or ethanol. The resulting crystals are grown into parallelepiped shape with well-defined facets in less than a few minutes after dropping the solution on a solid substrate at ambient condition. We expect that our novel method would contribute to the growth of other molecular crystals applicable in various fields.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-75**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Control of Molecular Crystal Growth Pathway by Reversing Solvent Addition Order

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

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

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

To obtain organic molecular crystals with controlled morphologies and crystal structures, conventional anti-solvent crystallization (c-ASC) process has been widely used by introducing anti-solvent into the original homogeneous solution to induce the target molecules nucleation and growth into crystals through the creation of supersaturation environment, which influences nucleation process and thus determines both morphology and crystal structure of the resulting crystals. During the c-ASC process, the supersaturation environment regarded intrinsic and invariable unless the kind and amount of target solvents are significantly varied. In this presentation, we present that the modified c-ASC process (reverse-ASC, r-ASC process) by simply reversing the solvent addition order induces dramatic changes in the crystallization, resulting in molecular crystals of organic molecules having unprecedented morphology. Specifically, We obtained zinc tetra(4-pyridyl) porphyrin (ZnTPyP) cube crystals by the r-ASC process that is formed by stacking of 2D ZnTPyP coordination polymer with toluene using as anti-solvent.¹ Different from the conventional attempt to crystallize molecules in solution by the c-ASC method that results in precipitates without specific morphology, The ZnTPyP cube crystals were prepared by adding good solvent into a prepared precursor solution in an anti-solvent (In this work, an excess amount of ZnTPyP was dispersed in toluene as anti-solvent, then, isopropanol as good solvent was added later). To explain the mechanism of the phenomena, we propose the extended first solvation shell effect (extended FSSE) mechanism, which elucidates that the solvent added first makes the most significant effect on the local supersaturation environment, determining the probable kinetic route that could not be chosen during the c-ASC. We believe that this work would grant an opportunity not only to study fundamentals of crystallization but also to control their crystal shapes. Reference 1. Park, Y.; Hong, M.;

Koo, J. Y.; Lee, M.; Lee, J.; Moon, D. J.; Sohn, S. H.; Joo, T.; Lim, W. T.; Lim, H.; Choi, H. C. *Sci. Rep.* 2017, 7, 2582.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-76**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly reproducible Formation of potassium-doped picene single crystals by enhancing diffusion of alkali metal by double diffusion method

Jinho Lee, Hee Cheul Choi*

Department of Chemistry, Institute for Basic Science, Korea

In this presentation, we present a newly developed double diffusion method to make uniform and reproducible alkali metal doping into picene single crystals to make them into molecular superconductor. By changing the sample temperature during the doping process, we achieved intercalation of alkali metal into small space in the picene single crystal having closed packed crystal structure, promoting the diffusion of dopants to result in uniform doping. Based on the optical microscopic observation and Raman spectroscopy, we confirmed the resulting samples are uniformly doped K_2 picene single crystals. Our in-situ electrical conductivity and resistance-temperature relation measurements revealed that insulator-to-semiconductor transition occurs upon doping. however, the crystal does not become fully metallic, as also predicted by previous theoretical studies [1-2]. After the doping process is completed, the doped picene did not show KH- and KOH-related peaks in X-ray diffraction (XRD), indicating a successful synthesis of high-quality doped samples without decomposition of the picene backbone molecules. We believe that our novel doping method for alkali-metal-doped molecular single crystals may provide better chances to design and fabricate them into high quality devices to study their electrical properties, through which the origin of superconductivity could be elucidated and eventually providing a facile and reliable way for the discovery of novel organic superconductors. References[1] *Phys. Rev. B* 2010, 82, 195114.[2] *Phys. Rev. B* 2014, 90, 075143.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-77

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Rapid, Resist-free Patterned Growth of Sea-Urchin-Shaped Hierarchical Porous Covalent Organic Framework-5 (COF-5) by Photochemical Synthesis Method

soyoung kim, Jung Jaehoon¹, Hyunseob Lim^{2,*}, Hee Cheul Choi^{*}, Yousoo Kim³

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

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²*Department of Chemistry, Chonnam National University, Korea*

³*Surface and Interface Science Laboratory, RIKEN, Japan*

Long reaction time and high reaction temperature, two significant shortages in the conventional solvothermal synthetic method for covalent organic frameworks(COFs), were overcome by a novel photochemical synthesis method. In this presentation, we present the rapid and patternable photochemical synthesis of covalent organic framework-5 (COF-5) using two types of ultraviolet (UV) light sources in a very short reaction time (~ 1h) with high yield (~90 %). The photochemically obtained COF-5(UV-COF-5) has hierarchical, homogenous “sea-urchin” shape morphology which is responsible for the superior gas adsorption property due to their high surface area. Theoretical calculations suggest that the orbital coupling between COF-5 layers at electronically excited state is related to the enhanced growth rate along the out-of-plane direction, leading to the formation of one-dimensional tentacle-like structures. In addition, we successfully achieved the spatially controlled growth of COF-5 by simply using reusable optical masks without any complicated lithographic or post-synthesis etching process. We believe that our findings would contribute to the development of novel strategies for the synthesis of various COFs and provide a great opportunity for their utilization in electronic and optoelectronic applications.¹ S. Kim, C. Park, M. Lee, I. Song, J. Kim, M. Lee, J. Jung, Y. Kim, H. Lim, H. C. Choi, *Adv. Funct. Mater.* 2017, 1700925

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-78**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of 1,1-Diisopropyl(or 1,1-Diphenyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)siloles and their applications to Lithium-ion battery

Yoon-ho Cho, Young Tae Park*

Department of Chemistry, Keimyung University, Korea

1,1-Diisopropyl(or 1,1-Diphenyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)siloles were prepared by the intramolecular reductive cyclizations of diisopropyl(or diphenyl)bis(phenylethynyl)silanes with treatment of 4.5 mol lithium naphthalenide and followed by 4 mol chlorotrimethylsilane solution in THF¹. After the reaction was finished, the naphthalene was removed via naphthalene sublimation apparatus, and the crude product was purified by recrystallization. The obtained materials are soluble in usual organic solvents such as THF and CHCl₃. The prepared materials were characterized by NMR, and IR spectroscopies. We also studied the electronic properties of the prepared silole derivatives by UV-vis absorption, excitation and fluorescence emission spectroscopic methods², in particular. In order to study the electrochemical properties of the synthesized materials, we also prepared a composite of the obtained carbosilanes with silicon nano powder, and examined the characteristics as a lithium-ion battery³.References:1. K. Tamao, S. Yamaguchi, and M. Shior, *J. Am. Chem. Soc.* 1994, 116, 11715.2. Y. T. Park, *Bull. Korean Chem. Soc.* 2016, 37, 56.3. Y. M. Jung, S-H Baek, and Y. T. Park, *Bull. Korean Chem. Soc.* 2017, 38, 91.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).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-79**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Interpenetrated 2D and 3D Ag(I) Coordination Networks Involving Nitrile-type Ligand

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Department of Chemistry, Gyeongsang National University, Korea

¹*Research Institute of Natural Science, Gyeongsang National University, Korea*

In the development of silver(I) coordination polymers, numerous dipyriddy-type ligands as nitrogen donor ligands have been intensively employed. Despite the rapid growth in the Ag(I) coordination chemistry, however, nitrile-type ligands (containing cyano groups) have been comparably ignored. In this sense, p-phenylenediacetonitrile as a nitrile-type ligand was chose for the development of Ag(I) coordination polymers with fascinating properties and interesting topologies. Reaction of p-phenylenediacetonitrile (L) with AgX (X = ClO₄ and PF₆) afforded two kinds of Ag(I) coordination networks with the same composition of {[Ag(L)₂]⁺X_n}. The perchlorato compound shows three-fold interpenetrated 2D network (Fig. 1a), while the hexafluorophospato compound displays an infinite three-fold interpenetrated 3D network (Fig. 1b). Herein, we report the crystal structures of both networks, the role of anions, and the difference of the conformation of nitrile-type ligand in the formation of 2D and 3D networks.

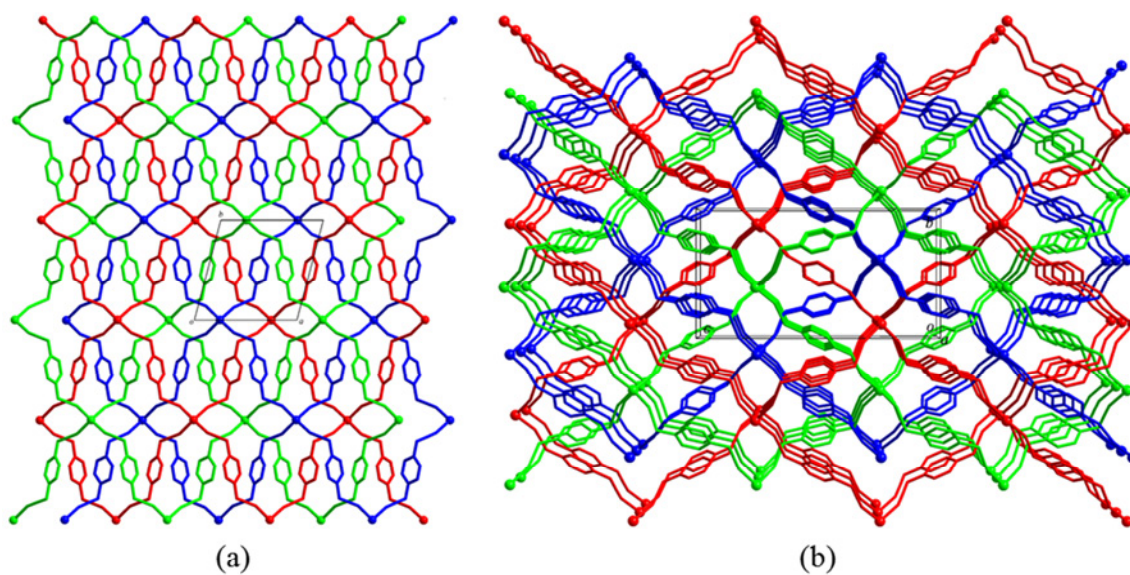


Fig. 1. Three-fold interpenetrated (a) 2D and (b) 3D Ag(I) coordination networks



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-80**

Area: Inorganic Chemistry

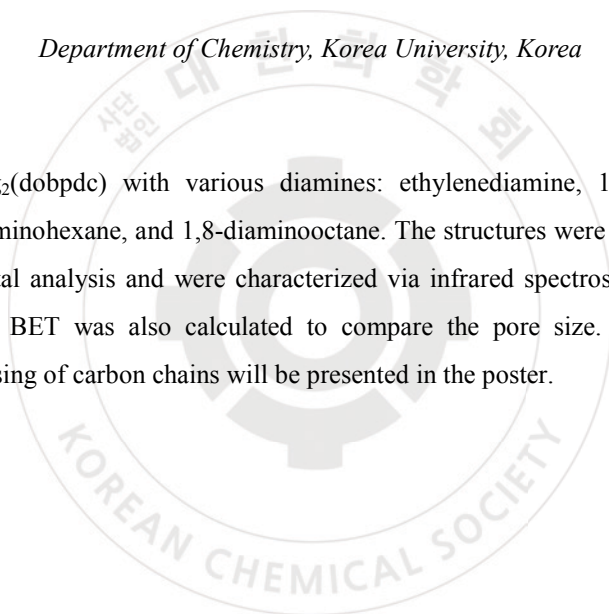
Type: Poster Presentation, Time: THU 11:00~12:30

Diamine with different alkyl lengths Functionalization of Mg₂(dobpdc)

**Jong Hyeak Choe, Hwa Young Lee, Jeong Hwa Song, Dongwon Kang, Hangeul LEE,
Jeong eun KIM, MINJUNG KANG, Sunhui EOM, Chang Seop Hong***

Department of Chemistry, Korea University, Korea

We functionalized Mg₂(dobpdc) with various diamines: ethylenediamine, 1,3-diaminopropane, 1,4-diaminobutane, 1,6-diaminohexane, and 1,8-diaminooctane. The structures were identified via powder X-ray diffraction, elemental analysis and were characterized via infrared spectroscopy, thermogravimetric analysis, and sorption. BET was also calculated to compare the pore size. Detailed properties and tendency toward increasing of carbon chains will be presented in the poster.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-81**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Generation of Nanoporous Copper (I) Silicate from Copper (II) Silicate, SGU-29

DONG HYEON LEE, Hyun Sung KIM^{1,*}

Department of chemistry, Pukyong National University, Korea

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

Originally, transition metal oxide molecular sieve, SGU-29 contains square plane-oxygenated Cu(II) active site. We developed novel strategy for chemical reducing Cu(II) to Cu(I) in SGU-29 framework without structural damage. Consequently, for the first time, generation of microporous of Cu(I) molecular sieve having SGU-29 structure has been achieved. Also we could reversibly oxidize Cu(I) to Cu(II) in SGU-29 framework without structural damage. This finding will expedite that the Cu(I) sensitively affects the behavior of microporous transition metal oxide molecular sieve such as selective toxic gas sorbent and heterogeneous catalytic application.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-82**

Area: Inorganic Chemistry

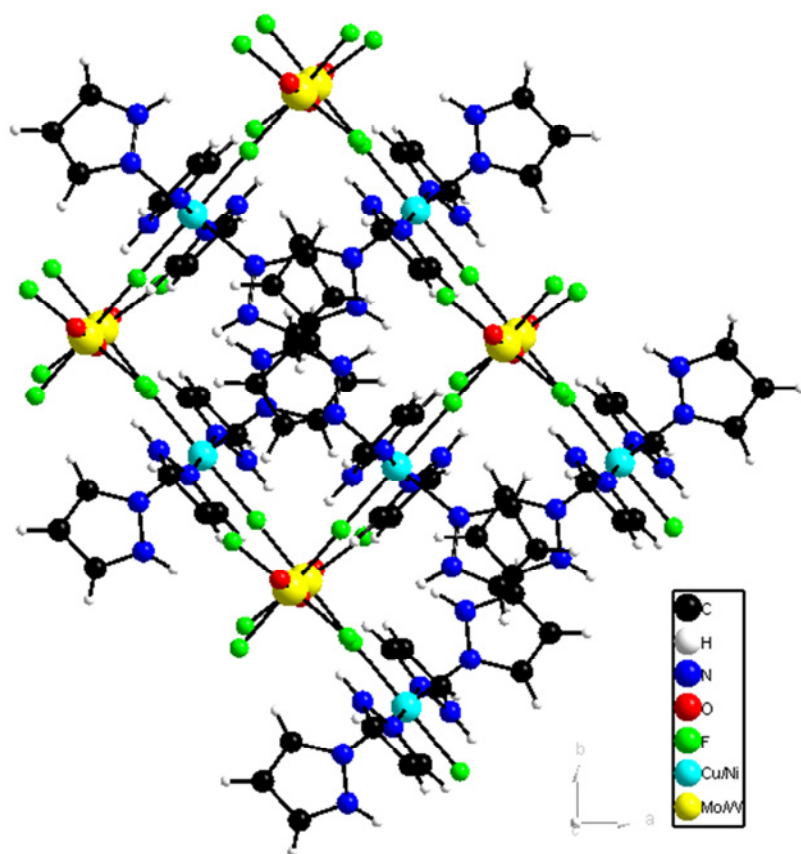
Type: Poster Presentation, Time: THU 11:00~12:30

Novel pyrazole molybdenum oxyfluoride compounds

Belal Ahmed, EunJeong Cho, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

In oxyfluoride chemistry, the octahedral basic building units, $[\text{MO}_x\text{F}_{(6-x)}]^{2-}$ (M = transition metals) are interesting because they are normally used to design noncentrosymmetric materials with magnetic properties. A new route is described to successfully synthesize four mixed metal oxyfluorides, $[\text{M}'(\text{pyrazole})_4][\text{MO}_2\text{F}_4] \cdot y\text{H}_2\text{O}$ (M' = Cu, Ni; M = Mo, W; and y = 0.10, 0.70, 1.78) using the combination of acentric units, $[\text{MO}_2\text{F}_4]^{2-}$ and $[\text{M}'(\text{pyrazole})_4]^{2+}$ by hydrothermal reactions. All the compounds crystallize in monoclinic crystal space group, *C2/c*. The $[\text{MO}_2\text{F}_4]^{2-}$ unit in the reported compounds exhibits *trans* directing properties with direct coordination through two *trans* F⁻ or one O²⁻ and one F⁻ ligands owing to the large nucleophilicity of ligands and the significant π -bonding between Mo/W and oxide ligands. Structures of all the synthesized compounds are well characterized by using thermal analysis, spectroscopic methods as well as elementary analysis.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-83**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

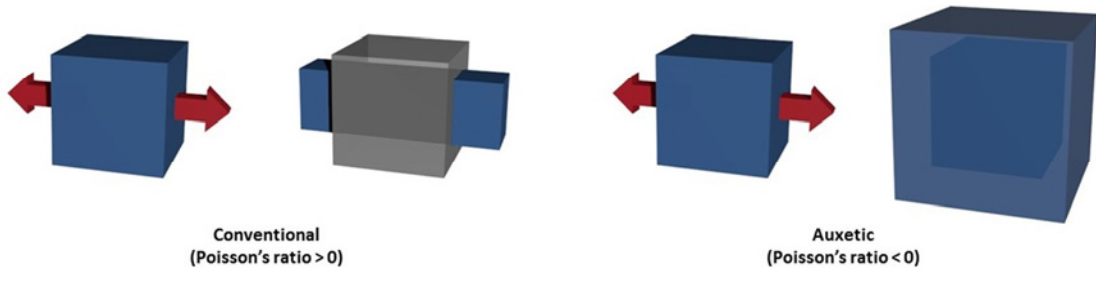
Radially Expandable Metal-Organic Framework with anomalous behaviour

Eunji Jin, Dongwook Kim, Woo-Dong Jang¹, Myoung Soo Lah, Seung Kyu Min, Wonyoung Choe^{*}

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

¹Department of Chemistry, Yonsei University, Korea

Auxetics, which are materials with negative Poisson's ratio (NPR), rarely found in natural and artificial materials, and known to be potentially useful in new applications. Interestingly, such auxetics can be rationally designed based on geometric models. Metal-organic frameworks (MOFs), a new class of solid-state materials can be an ideal platform for auxetic crystalline materials because of their structural tunability from various structural components. Despite of such merits unique to MOFs, discovery of MOF auxetics have been a daunting challenge to date. Herein, we report a flexible porphyrinic MOF (UNIST-Porphyrin Framework-1, UPF-1), which demonstrates simultaneous colossal thermal expansion and auxetic behaviour. Single crystal and powder X-ray diffraction analysis and simulation indicates that the abnormal mechanical properties are caused by the cooperative movement of internal hinged SBUs in UPF-1. Similar to zeolites, the geometric model of UPF-1 follows the rotating rigid cube model of auxeticity. This work demonstrates that topology of the framework and flexible hinges inside the structure are intimately related to mechanical properties, providing a guideline for rational design of new series of NPR MOFs.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-84**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Syntheses and Structural studies of Metal Complexes with Ligand derived bis(ethylamine)

JongWan Lim

Chemistry, Simin High School, Korea

.Syntheses and Structural studies of Metal Complexes with Ligands derived bis(ethylamine)The ligands were synthesized by a reaction of 2,2'-(ethylenedioxy)bis(ethylamine) with salicylaldehyde or 3,5-dimethylpyrazolylmethanol. We synthesized nickel complexes with N,N'-disalicylidene-2,2'-(ethylenedioxy)bis(ethylamine)(H₂dee), and determined the crystal structure of the isolated complex, which show a unique dinuclear core with two phenolated-oxygen bridges and the μ -aqua bridge. Cobalt complexes of N,N',N',N'-tetra-[(3,5-dimethyl-1-pyrazolyl)methyl]-2,2'-(ethylenedioxy)bis(ethylamine) were synthesized.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-85**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solvothermal Synthesis and Structural Characterization of (MeNH₃)₂[Pd(Se₄)₂]·Se₈

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department of chemistry, Incheon National University, Korea

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

Pd polyselenides are famous to be highly sensitive to the change in cations and result in various compounds with novel structures. A smallest organic cation, MeNH₃⁺ was employed for the first time in the Pd polyselenide system. (MeNH₃)₂[Pd(Se₄)₂]·Se₈ was successfully synthesized by the solvothermal method using methanol as a solvent. Crystal structure of (MeNH₃)₂[Pd(Se₄)₂]·Se₈ was determined by the single crystal X-ray diffraction study. Black polyhedral crystals of (MeNH₃)₂[Pd(Se₄)₂]·Se₈ crystallize in the tetragonal space group P-4b2 (no. 117) with $a = 12.7821(4) \text{ \AA}$, $b = 12.7821(4) \text{ \AA}$, $c = 7.1123(2) \text{ \AA}$, $V = 1162.02(8) \text{ \AA}^3$. (MeNH₃)₂[Pd(Se₄)₂]·Se₈ was found to possess a layered Pd polyselenide anion, Pd(Se₄)₂²⁻ with encapsulated Se₈ rings as it become the structural analog of A₂[Pd(Se₄)₂]·Se₈ (A = Rb, Cs). We had attempted the removal of MeNH₃⁺ organic cation from (MeNH₃)₂[Pd(Se₄)₂]·Se₈ without the loss of structural integrity by thermal decomposition and examined (MeNH₃)₂[Pd(Se₄)₂]·Se₈ before and after thermal decomposition by SEM, XRD and BET measurements.

Conference Date: October 18~20, 2017

Venue: Kimdajejung Convention Center, Gwangju

Code: **INOR.P-86**

Area: Inorganic Chemistry

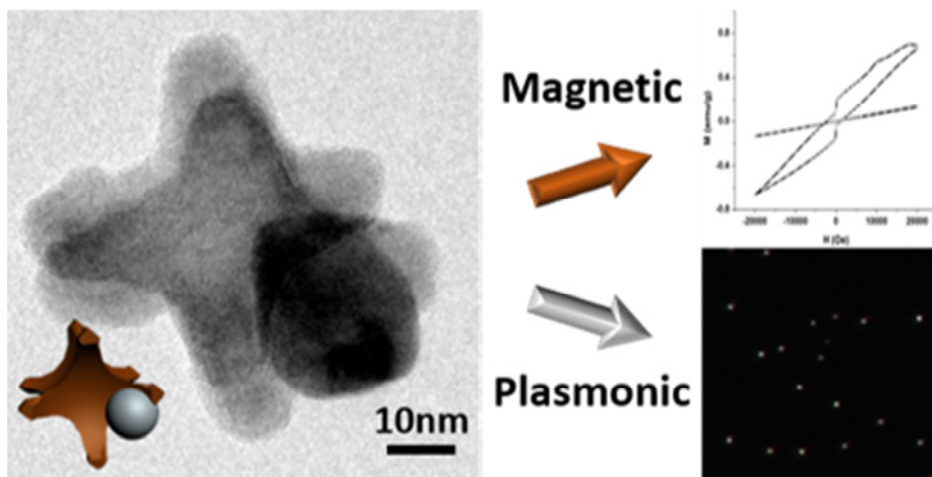
Type: Poster Presentation, Time: THU 11:00~12:30

Selective Growth and Structural Analysis of Octapod MnO and Ag-octapod MnO Hybrid Nanostructures for Imaging Probes

Dongwoo Shin, Hyunjoon Song*

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

MnO–Ag heterodimers have been synthesized by the growth of Ag domains using a phase-transfer protocol in toluene. The Ag domains were directly attached to one of the concave faces with high index facets, dominantly (533), of the MnO octapods. The resulting MnO–Ag heterodimers have basically two independent domains. On this basis, multiple functions are expected, including plasmon light scattering from the Ag domains and magnetic resonance from the MnO domains. Notably, the heterodimers strongly scattered visible light at 420 nm, and even a single particle signal could be detected in a dark-field spectroscopy image. The scattering peak was extended to the near-IR range by the formation of MnO octapod–AgAu hollow heterodimers via a galvanic replacement reaction. The heterodimers also showed weak ferromagnetism at low temperature, and exhibited a positive T1 signal in magnetic resonance imaging. These properties demonstrate that the MnO–Ag heterodimers can potentially serve as dual imaging probes for biological systems.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-87**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

New Zr-based MOF with Spirobifluorenetetrabenzoic Acid as an Efficient Catalyst for the Hydrolysis of a Nerve Agent Simulant

Hea Jung Park, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

Detoxification of highly toxic chemical warfare agents is starting to attract attention as a matter of great importance. Recently, MOF-based hydrolysis of nerve agent simulant is of considerable interest. New microporous zirconium(IV)-based metal-organic framework (MOF) containing 4,4',4'',4'''-(9,9'-spirobi[fluorene]-2,2',7,7'-tetrayl)tetrabenzoic acid, namely Spirof-MOF has been synthesized and characterized for this purpose. It exhibited BET surface area of 2017 m²g⁻¹ and two types of diamond-shaped channels along the *a*- and *c*-axis with 6 Å and 8 Å aperture diameters, respectively. Synthesized Spirof-MOF has been employed as a catalyst for the hydrolysis of nerve agent simulant DMNP. Among the three prepared Spirof-MOF samples, size controlled Spirof-MOFb showed 99% conversion over the course of 18 min and fastest half-life (50% conversion, *t*_{1/2}) of 1.8 min among the Zr-based MOF containing 8-connected Zr₆-cluster node (hydrated).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-88**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Demonstration of Efficient Energy Transfer (ET) within the Pyrene and Porphyrin-Based Mixed Ligands Metal-Organic Frameworks

Kyoung Chul Park, Yoo Eil Jung, Chang Yeon Lee*

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

Solvothermal reaction between the Zr_6 cluster and mixture of an appropriate ratio of 1,3,6,8-tetrakis(p-benzoic acid)pyrene (H_4TBAPy) and [5,10,15,20-Tetrakis(4-carboxy-phenyl)porphyrinato]-Zn(II) (Zn-TCPP) provided the mixed-ligand MOFs (MLMs, MLM-1~3). Due to the identical symmetry and connectivity of the two ligands, MLMs were successfully synthesized as a single MOF form. Efficient energy transfer (ET) between two ligands in MLMs would be expected because of the good overlap between the emission spectrum of pyrene and the absorption spectrum of porphyrin. This expecting phenomenon was confirmed by the confocal fluorescence mapping and fluorescence lifetime mapping techniques carried out with the nanoscale spatial resolution. Moreover, MLMs were employed as a photoinduced singlet oxygen generator to verify their enhanced light-harvesting properties. MLMs exhibited the superior performances for singlet oxygen generation compared with those of comparative test subjects. The enhancement of light-harvesting through the complementary absorption and energy transfer between two ligands in MLMs is responsible for the increase of photoinduced singlet oxygen production ability. Acknowledgment : 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 (NRF2016R1A2B4010376)

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Code: INOR.P-89

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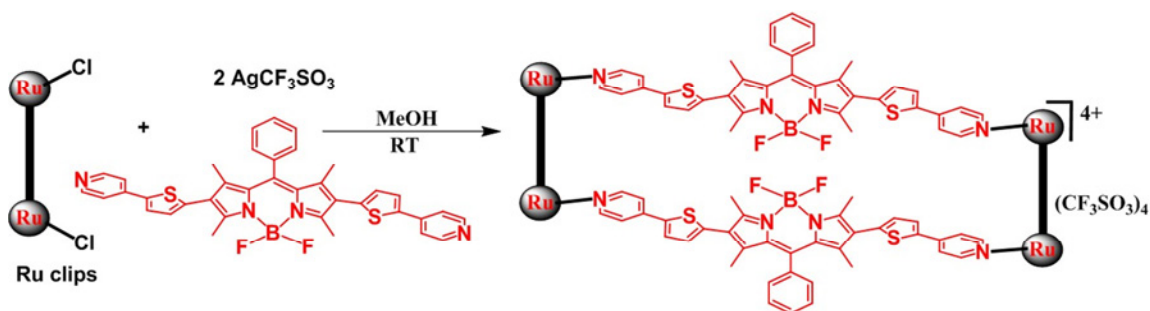
Type: Poster Presentation, Time: THU 11:00~12:30

Self-Assembly of Novel Thiophene-based BODIPY Ru(II) Rectangles

GAJENDRA GUPTA, Jung Suk Oh, Jungwon Park, Chang Yeon Lee*

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

New thiophene-functionalised dipyrindyl BODIPY ligand has been designed and utilised for the synthesis of (2+2) metalla-rectangles by self-assembly. The synthesized complexes are fully characterized by different analytical techniques including single crystal XRD structures for representative complexes. The complexes exhibited dose-dependent antiproliferative activities against cancer cells. The characteristic green fluorescence of the BODIPY ligand in these supramolecules permits intracellular visualization of complexes using confocal microscopy, and detects the localization of the compounds in the cytoplasm and on the plasma membrane. Moreover, the supramolecules also displayed substantial propensity to bind with biomolecules which could be the probable reason for its high activity. Acknowledgment : 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 (NRF2016R1A2B4010376)



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-90**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Hollow MoS₂/C Composites using Yolk-Shell PS@Microporous Organic Network for High Performance Pseudocapacitors

Hyunjae Lee, Jaewon Choi¹, Seung Uk Son^{1,*}

Chemistry, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

We designed and synthesized yolk-shell type PS@microporous organic network (Y-PS@MON). While yolk PS is nonporous, shell MON has a high surface area and microporosity. Thus, precursors can be incorporated into Y-PS@MON. The inner yolk PS is gradually disassembled through heat treatment. Thus, Y-PS@MON showed the efficient engineering of hollow inorganic material/carbon composite materials. MON materials are a recent class of porous organic materials. The MONs have shown high surface areas and microporosities. This presentation shows new material chemistry of MON materials. As far as we are aware, yolk-shell MON materials have not been reported. Compared to inorganic materials, the engineering of organic templates has been relatively less explored. Especially, porous organic templates are rare, while non-porous polymer beads have been used as templates. Many scientists have made efforts to improve storage capacitances of supercapacitors. RuO₂ materials with pseudocapacitive property and a high theoretical capacitance gave an impressive impact as energy storage materials for supercapacitors. However, RuO₂ is a very expensive material. Recently, MoS₂ with pseudocapacitive property (theoretical capacitance up to ~ 1000 F/g) has attracted attention in the field of supercapacitors. While MoS₂ only shows poor performance due to its low conductivity and facile stacking behavior, the appropriate distribution of MoS₂ materials over carbon matrix can realize promising electrochemical performance. For this, the efficient engineering of Mo₂/C composites is critical. In our work, Y-PS@MON materials resulted in the efficient engineering of hollow MoS₂/C composites. Moreover, the contents of MoS₂ in the composites were systematically controlled. In symmetrical coin cell (CR2032) supercapacitors, the optimal MoS₂/C-58 composites showed high specific capacitances up to 418 F/g at a

0.5 A/g current density, rate performances with 235 F/g at a 10 A/g current density, and cycling stabilities during 5000 cycles.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-91**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fluoropolymer Stabilized Chromophore-Catalyst Assemblies in Aqueous Buffer Solutions for Water Oxidation Catalysis

Kyeong Min Lee, Kyung-Ryang Wee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

We describe here application of the fluorinated polymer (Dupont AF, a copolymer of 4,5-difluoro-2,2-bis(trifluoromethyl)-1,3-dioxole and tetrafluoroethylene) as the overlayer in stabilizing phosphonate-derivatized molecular assemblies on mesoporous metal oxide electrodes. In the procedure, the polymer is dip coated onto the surfaces of oxide electrodes with pre-bound, phosphonate-derivatized chromophores and assemblies including assemblies for water oxidation. With water as the solvent, a troublesome arises from loss of surface-bound chromophores and catalysts due to desorption and decomposition from the metal oxide surface. Especially, desorption and decomposition is occurred under basic conditions. We compare here PMMA method previously reported with AF polymer property. The results of our experiments demonstrate a high degree of stabilization by the added polymer and a demonstration of its use in stabilizing surface-bound assemblies for water oxidation catalysis in aqueous solutions by CV data.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-92**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

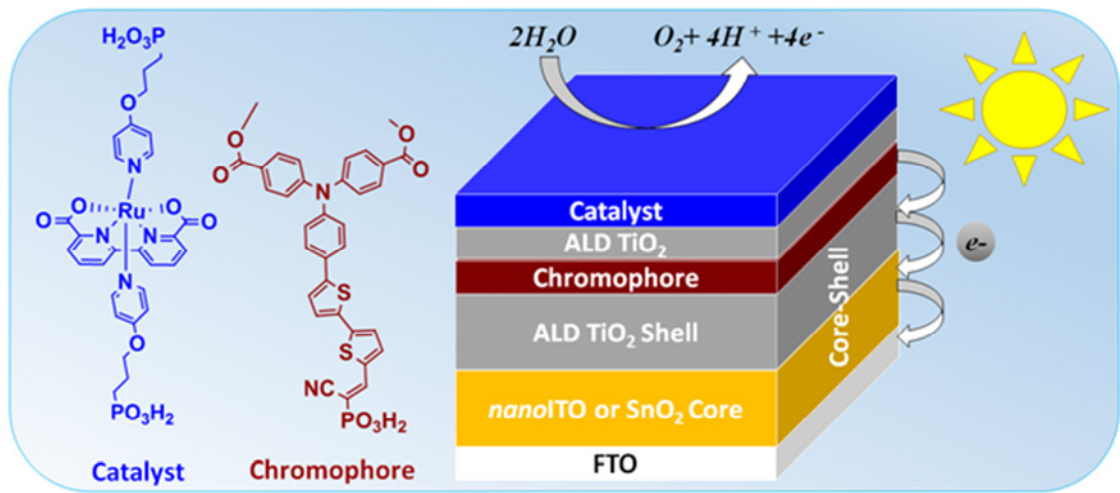
Chromophore-Catalyst Assembly for Visible-light driven water oxidation prepared by Atomic Layer Deposition

gunoh bae, Kyung-Ryang Wee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

Visible-light-driven water splitting was investigated in a dye sensitized photo-electrosynthesis cell (DSPEC) based on a photoanode with a phosphonic acid-derivatized donor- π -acceptor (D- π -A) organic chromophore, 1, and the water oxidation catalyst [Ru(bda)(4-O(CH₂)₃P(O₃H₂)₂-pyr)₂], 2, (pyr = pyridine; bda = 2,2'-bipyridine-6,6'-dicarboxylate). Each photoanode was prepared by using a layering strategy beginning with the organic dye anchored to an FTO|core/shell electrode, atomic layer deposition (ALD) of a thin layer (< 1 nm) of TiO₂, and catalyst binding through phosphonate linkage to the TiO₂ layer. Device performance was evaluated by photocurrent measurements for core/shell photoanodes, with either SnO₂ or nanoITO core materials, in acetate-buffered aqueous solutions at pH 4.6 or 5.7. Although the absolute magnitudes of photocurrent changes with the core material, TiO₂ spacer layer thickness, or pH, observed photocurrents were 2.5-fold higher in the presence of catalyst. Results of transient absorption measurements and DFT calculations reveal that although electron injection by photo-excited organic dye is ultrafast, recombination is nearly 95% complete by 1.5 ns arising from the orientation of the dye's molecular orbitals on the oxide surface. Although chromophore decomposition does occur which limits efficiency, O₂ evolution is observed from these photoanode assemblies which combine ease of assembly with surface stability.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-93**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Organic Dye Chromophore Stability on Nanocrystalline Metal Oxide Surface in Aqueous Solution for Dye-Sensitized Photoelectrochemical Cell

Mina Ahn, Kyung-Ryang Wee^{1,*}

Department of Chemistry, Daegu University, Korea

¹*Department of Applied Chemistry, Daegu University, Korea*

The oxidative stability of a donor- π -acceptor (D- π -A) organic dye, consisting triphenyl amine, bithiophene, and carboxylate (C-A- π -D) or phosphonate (P-A- π -D and PP-A- π -D) anchoring unit, on nanocrystalline TiO₂ surfaces in various aqueous system toward both electrochemical and photoelectrochemical oxidation are described. Electrochemical measurements on the dye on TiO₂ in various pH reveal scan rate dependent oxidations for the -[P-A- π -D]^{+/₀} and -[P-A- π -D]^{2+/₊} couples with the latter chemically reversible at scan rates >400 mV/s. Photostability of FTO|nanoTiO₂-[P-A- π -D] electrodes under illumination with injection into TiO₂ and back electron transfer occurring on the surface is surface coverage dependent with the highest stability achieved for completely loaded surfaces with close packing of the -P-A- π -D molecules creating a self-protecting hydrophobic film effect. There are various methods about stabilization of organic dye chromophore on the surface such as atomic layer deposition (ALD) over layer and polymer over layer. In the ALD over layer, organic dye shows no enhanced electrochemical stability by ALD over layer protection, and moreover ALD accelerate organic dye decomposition. In the polymer over layer, organic dye shows enhanced electrochemical stability and stabilized the surface bounding.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-94**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Syntheses, structure and characterization of Copper (II) (ebpp)₂ complex having NO_x attachment

Mohammad Sherjeel Javed Khan, jang hoon Cho, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

The chemistry of transition-metal-NO complexes, or metal nitrosyls, has taken on added significance in recent years because of the important role that nitric oxide has been found to play as a signaling molecule in biological systems. Recent work has also established that the characteristic chemistry of nitrosyl complexes is often markedly different from that exhibited by their isoelectronic carbonyl analogues. Copper containing enzymes play a central role in denitrification, whereby bacteria use NO₃ and NO₂ as terminal electron acceptors, ultimately producing NO, N₂O, and/or N₂. A copper-NO species has been proposed as a key intermediate in biological nitrogen oxide reduction, and NO adducts of other copper system have been proposed. In this study, we have developed a copper complex by using spontaneous self-assembly of an organic ligand and Cu(II) ion to investigate the mechanistic details of the nitrosyl activity of the complex by using IR, Raman, UV visible and EPR techniques.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-95**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Stepwise modification of the Zn₄O clusters in MOF-5 for enhanced CO₂ and CH₄ gas adsorption

NAKEUN KO, Jaheon Kim^{1,*}

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

¹*Department of Chemistry, Soongsil University, Korea*

MOF-5 is a highly porous metal-organic framework (MOF) formulated as Zn₄O(BDC)₃ (BDC = benzene-1,4-dicarboxylate) but exhibits little gas adsorption selectivity due to the absence of strong adsorption sites. To overcome these disadvantages, we have replaced the Zn ions of the Zn₄O clusters partially with octahedral Ni ions to which bidentate ligand can be attached. Next, to the modified MOF (Ni/Zn-MOF-5-L), another metal ions have been incorporated to give Ni/Zn-MOF-5-L-M. Although Ni/Zn-MOF-5-L-M shows a significantly decreased surface area, it can absorb CO₂ or CH₄ than MOF-5 itself by more than 50 % at 273 K probably due to the introduced metal ions (M) and their role as open-metal sites. Interestingly, Ni/Zn-MOF-5-L-M has more enhanced moisture stability than pristine MOF-5.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-96**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

High-throughput screening for Zn- and Cd-ZIFs exhibiting SOD or RHO topology in mixed-solvent systems

Yejin Choi, hakyung yun, Jaheon Kim^{*}

Department of Chemistry, Soongsil University, Korea

Unlike zeolites, the framework types of zeolitic-imidazolate frameworks (ZIFs) are known to be determined by the steric factors originating from bonded functional groups to an imidazole backbone. To find out other structure-directing factors, we have conducted high-throughput solvothermal reactions with a selected imidazole (2-nitroimidazole) and Zn(II) or Cd(II) ions with employing designed solvent systems in which different solvents were mixed in various ratios. The resulting products were mainly ZIF-sod or ZIF-rho based on X-ray diffraction analysis. Here, by analyzing solvent-product maps obtained from the high-throughput reactions, we propose the relationship between the obtained structures and used solvent systems.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-97**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Attachment of amino acids to the organic linkers in metal-organic frameworks

Kyungkyou Noh, YOU JIN OH¹, Jaheon Kim^{1,*}

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¹*Department of Chemistry, Soongsil University, Korea*

We have studied how to introduce amino acids (AAs) to metal-organic frameworks (MOFs). For example, we conducted coupling reactions of five selected amino acids with the organic linkers in MIL-101 to give MIL-101-[AA]s and examined the reactivity of each amino acid based on ¹H-NMR measurements. The MIL-101-[AA]s were, in turn, reacted with another AAs to form MIL-101-[AA]-[AA]. Also, we attached non-AA spacer molecules to MIL-101 first, and the introduced spacers were reacted with AAs to give MIL-101-[spacer]-[AA]s. The synthesis, characterization, and potential applications of the AA-decorated MOFs will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-98**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facile synthesis of Al-MOFs in basic aqueous solution

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¹*Department of ICMC convergence technology, Soongsil University, Korea*

Metal-organic frameworks (MOFs) composed of Al ions and organic carboxylates are usually stable in water thereby Al-MOFs are candidates for water adsorbents in heat-driven chillers. Previously, we could prepare 2 kg of Al-fumarate at room temperature simply mixing reactions in aqueous NaOH solution. The water uptake property of the Al-fumarate products was dependent on the concentration of NaOH. We applied this simple method to the preparation of other Al-MOFs such as MIL-53 and CAU-10 and analyzed the crystallinity, porosity, and water adsorption properties, which will be discussed in this presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-99**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Application of Imidazolium- Based MOFs

Jaechul Lee, Kyungkyou Noh¹, Jaheon Kim², Kimoon Kim, Eunsung Lee*

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

¹*Department of ICMC convergence technology, Soongsil University, Korea*

²*Department of Chemistry, Soongsil University, Korea*

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 emerging for some applications such as proton conductor or N-heterocyclic carbene (NHC) precursor. However, one of the major problems on the imidazolium-based MOFs was its poor stability. To solve this problem, we designed new imidazolium ligands with pyrazolate as the metal binding group which is well known to form strong metal to ligand bond even stable under basic condition. From this ligand, series of new imidazolium MOFs were successfully synthesized. The properties and potential applications of these materials will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-100**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

1D-Copper aconitate compounds and its conformational change by UV irradiation

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¹*Department of Chemistry, Konkuk University, Korea*

Metal-organic polymer chemistry is an important research topic due to the variety of the composition and topology of the produced compounds, and also to their interesting functional properties and potential applications for catalysis, molecular storage, magnetism, electrical conductivity, sensor capability, luminescence, etc. In this work, three new compounds, [H₂-diaminopropane][Cu(Aco)(H₂O)]₂•5H₂O (1), [H₂-diaminobutane][Cu(Aco)(H₂O)]₂ (2), [H₂-diaminopropane][Cu(Aco)(H₂O)]₂•2H₂O (3) have been synthesized. These show 1D polymeric chain structures consisting of copper(II) and *trans*-aconitates(Aco) anion. The conformational change was observed in *trans*-aconitate by increasing temperature or the UV irradiation. The crystal structures of three compounds have been revealed by single-crystal X-ray diffraction techniques.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-101**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solvothermal investigation of Cu/muconic acid/phenethylamine system

Jaeun Kang, Junghwan Do*

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The new metal-organic coordination polymers, Cu(muconate)(phenethylamine) (1), Cu(muconate)(phenethylamine)₂ (2), [H-phenethylamine]₂[Cu₄(muconate)₅(phenethylamine)₂]·2(H₂O, ethanol) (3), have been synthesized and characterized by single-crystal X-ray diffraction techniques. These complexes were synthesized under mild solvothermal condition and show high dimensional structures (2D, 3D) with large pores. A long linear-shaped *trans,trans*-muconic acid containing two double C=C bonds is a good candidate as a linker molecule that could provide various network topology.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-102**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Au@CoS_x core-shell nanoparticle and its enhanced catalytic activity in hydrogen evolution reaction

Jun Kim, jisol park, Kwangyeol Lee^{*}

Department of Chemistry, Korea University, Korea

Up to date, hydrogen evolution reaction (HER) can be easily achieved via water electrolysis catalyzed by precious metals such as Pt, Pd and Rh. Nevertheless, the scarcity and high cost of noble metals impede their practical application in large scale, thus calling for the development of alternative, earth-abundant metal based materials with high electrocatalytic performance. Through substantial research efforts, a number of earth-abundant materials have been identified as promising candidates for HER electrocatalysts, including Co-based materials, namely cobalt chalcogenides. Herein, we report the synthesis of Au@CoS_x core-shell nanoparticle and its enhanced catalytic activity benefiting from Au core and amorphous nature of cobalt sulfide shell.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-103**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Seed-mediated formation of IrRu alloy nanocactus as bifunctional electrocatalysts for overall water splitting in acidic media

JOO JINWHAN, Haneul Jin, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The development of highly efficient and stable bifunctional electrocatalysts for overall water splitting in acidic media is necessary for polymer electrolyte membrane (PEM) electrolyzers, but it still remains a challenge due to several technical and experimental obstacles. While several non-noble metal catalysts are developed, they show short lifetime in acidic media. Herein, we report the preparation of cactus-like hollow $\text{Cu}_{2-x}\text{S}@{\text{IrRu}}$ nanoparticles which show high catalytic activity and stability for both hydrogen evolution reaction and oxygen evolution reaction in acidic condition. The initial formation of Ru-rich islands on pre-synthesized Cu_{2-x}S templates is followed by reduction of Ir and alloying, which is concomitant with the dissolution of the Cu_{2-x}S templates, as observed in the formation of the cactus-like $\text{Cu}_{2-x}\text{S}@{\text{IrRu}}$ structure.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-104**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Janus 2D structure controlling the anisotropic diffusion pathway dependent on crystal unit cell structure

jisol park, Jongsik Park, Kwangyeol Lee *

Department of Chemistry, Korea University, Korea

The synthetic methods of Janus structures have a great attention compared to alloy nanoparticles in terms of controlling their distinct electronic properties. According to the difference of surface energies between corners, edges and facets, the regiospecific hetero growth of nanostructures and unprecedented phase-segregated framework could be observed by using 3D nanostructural template. Through the selective protecting of nanostructure active sites, we could change the diffusion pathway of additional alloy formation. Herein, we demonstrate the unique diffusion pathway of additional alloy formation could be controlled dependent on their crystal unit cell structures.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-105**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Binary and Ternary Core-Shell Nanosandwich Structures with a Compositionally Tunable Core and Regio-Selectively Grown Shell

Taehyun Kwon, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Development of electrocatalysts with reduced noble metal content with enhanced catalytic performance has been of importance in cost-effective design of renewable energy conversion devices. The design of core-shell nanoparticle electrocatalysts represents a promising approach to developing catalytic activity as well as limiting the use of expensive precious metals. Herein, we report one-pot synthetic route to prepare hexagonal-shaped core-shell nanosandwich structure with compositionally tunable core and regio-selectively grown shell. The hexagonal core-shell nanosandwich structure possesses enhanced electrocatalytic activity toward oxygen evolution reaction (OER), with their OER activity being dependent on their core compositions.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-106**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of tetrahedral rhodium sulfide-based nanoframes as electrocatalysts for hydrogen evolution reaction

Minki Jun, Kwangyeol Lee^{*}

Department of Chemistry, Korea University, Korea

The effective hydrogen production is an essential prerequisite for hydrogen economy, and water electrolysis is a sustainable and clean method for hydrogen production, because it uses water as a feedstock. In order to supply cost-competitive hydrogen, highly active and robust electrocatalysts for hydrogen evolution reaction are required. Among the various catalysts structures, nanoframes has attracted considerable attention since its high catalytic surface areas and highly exposed edge sites. Herein, we demonstrate the simple synthetic scheme to prepare the rhodium sulfide-based nanocrystals with tetrahedral frame structures and its electrocatalytic activity toward hydrogen evolution reaction.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-107**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly porous PtNi multiframe nanocatalyst for oxygen reduction reaction

Hyukbu Kwon, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

As the depletion of fossil fuel becomes more serious worldwide, it is necessary to develop renewable, economical and green energy source. To satisfy these needs for alternative energy source, hydrogen energy system received attention and many researches revealed some noble metals especially Pt to be effective catalyst for boosting the rate determining reaction, oxygen reduction reaction(ORR). But low deposits and high price of Pt is deteriorating actual use of hydrogen as renewable energy source. Therefore, for effective and efficient use of Pt, series of researches were conducted on nano-scale structure and alloy composition with non-noble metals like Ni, Co, etc. because of its high surface to volume ratio and unparalleled catalytic activity. In this study, we report the synthesis of hierarchical hollow structure which is constructed by multiple stacked nanoframes. By adjusting the decomposition behavior of Pt and Ni precursor and applying chemical etching and thermal treatment, initially formed PtNi nanoparticle was converted to highly porous Pt₃Ni nanoframe. This alloy phase transition and structural evolution to have more open catalytic active sites boost its catalytic activity for ORR.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-108**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of mixed metal chalcogenides toward hydrogen evolution reaction by template-mediated method

Taekyung Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nanostructured metal chalcogenides have received a great attention in a variety of applications, which includes fuel cells, solar cells, supercapacitors, thermoelectric devices and sensors. Especially, ternary metal chalcogenides show a great promise due to their energy tunability and catalytic robustness under harsh operating condition. Template-mediated growth of nanoparticles is a very efficient method to synthesize well-defined colloidal nanocrystals because the template can be used as a platform where other materials are deposited by reduction or template components are released out by dissolution of template itself. In this research, we report a facile synthesis of ternary metal chalcogenides with well-defined structure prepared by template-mediated method toward hydrogen evolution reaction.

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Code: **INOR.P-109**

Area: Inorganic Chemistry

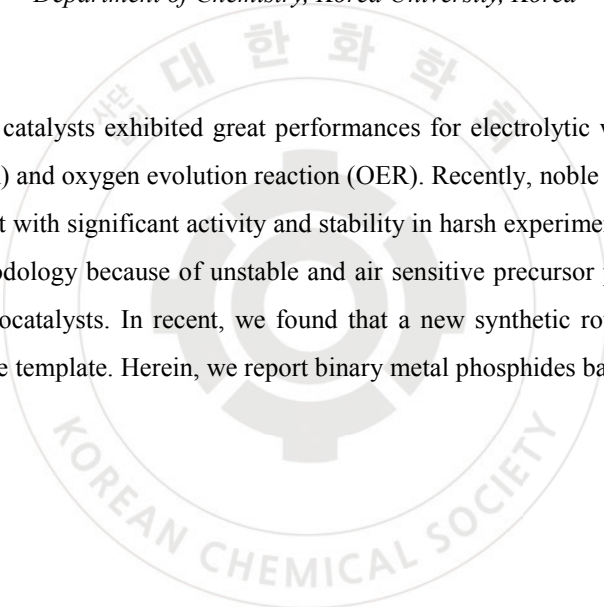
Type: Poster Presentation, Time: THU 11:00~12:30

Template mediated synthesis of noble metal phosphides

Haneul Jin, Kwangyeol Lee^{*}

Department of Chemistry, Korea University, Korea

Metallic semiconductor catalysts exhibited great performances for electrolytic water splitting; hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Recently, noble metal phosphide arose as a superior electrocatalyst with significant activity and stability in harsh experimental conditions. However, limited formation methodology because of unstable and air sensitive precursor permits only a few types of metal phosphide nanocatalysts. In recent, we found that a new synthetic route to make noble metal phosphide via metastable template. Herein, we report binary metal phosphides based on copper phosphide template.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-110**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Hemicore-shell as an optimal catalyst structure alloy@alloy nanoframe toward oxygen evolution reaction

SONGA CHOI, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The oxygen evolution reaction (OER) is a significant contributor to energy loss in proton exchange membrane (PEM) electrolyzers, and iridium based nanoframes with large surface area are well known as one of the most active electrocatalysts for OER. Since nanoframe-structured catalysts intrinsically have a problem that they are unstable during the catalysis, we suggest alloy@alloy core-shell nanoframe structures which show enhanced electrocatalytic activity arising from the surface strain via lattice mismatch between core and shell. Herein, we synthesized hemicore-shell and core-shell nanoframe structures to further improve the activity and durability of Ir-based nanostructures toward OER under acidic condition.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-111**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Hollow bimetallic phosphide nanocage: an efficient and durable electrocatalyst toward hydrogen evolution reaction

Yongju Hong, Jongsik Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Non-noble metal catalysts toward hydrogen evolution reaction (HER) have shown a tremendous development over the decades. Theoretical and experimental studies have proved the great catalytic performance of transition metal phosphides (TMPs), which is therefore considered as promising alternatives to noble metal-based catalysts. Furthermore, heterogeneous catalysis is gravely affected by high-energy structures such as grain boundaries and specifically exposed surface area which is the active sites of catalytic reactions. Recently, we found a facile route to prepare bimetallic nanoparticles with grain boundaries by aid of small amount of noble metal. Through further phosphidation, core component removed by Kirkendall effect, resulting in hollow bimetallic phosphide nanocages.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-112**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facet and phase controlled β -NiOOH nanocatalyst for oxygen evolution reaction

Byeongyoon Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Nickel oxide exists in β/γ -NiOOH phases during oxygen evolution reaction in alkaline condition. Even though β -NiOOH exhibits higher OER activity than γ -NiOOH, the β -NiOOH phase is inevitably oxidized to γ -NiOOH under OER working potential in alkaline aqueous solution. In this work, by using facet control of nanocrystal, we confined the hexagonal-close-packed nickel oxyhydroxide phase in crystal lattice of face-centered-cubic nickel oxide, and finally prevented the phase alteration and maintained the β -NiOOH electrode which is active and durable electrocatalyst for OER.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-113**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Photocatalytic CO₂ conversion on highly ordered mesoporous Materials

JOO JINWHAN, Kwangyeol Lee^{*}

Department of Chemistry, Korea University, Korea

Mesoporous materials are widely used in catalysts, batteries, sensors, and supercapacitors. Due to their large surface-to-volume ratio and 2-50 nm size pores, these materials have a great potential for various applications in energy field. Generally, mesoporous structures enhance diffusion of the reactants through channels, offering more active sites for reaction, which increase catalytic activity. In this study, hexagonally nano-wire arrayed catalysts are synthesized via the hard-template method. The SBA-15 silica template is prepared by soft template method and thermal annealing. The infiltration of precursors within the mesopores of silica template is followed by thermal treatment at high temperature. The highly ordered mesoporous materials are obtained by HF solution or NaOH treatment to remove the template. The photocatalytic CO₂ conversion result show that the nano-wire arrayed catalyst can convert CO₂ to CH₄ and CO under visible light irradiation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-114**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A New Co-based Metal-Organic Framework and Structure Based Magnetic Property Analysis

Jihyun Lee, Yoodea Song, Gyungse Park^{1,*}, Minyoung Yoon^{*}

Department of Nano Chemistry, Gachon University Global Campus, Korea

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

Despite its abundance of new metal-organic frameworks (MOFs), the synthesis of new MOFs is a still challenging issue in porous materials research field. Among the candidate metal ions, recently cobalt ions draw attention due to its unique spin state and catalytic activity. Herein, we present a new cobalt based MOF (Co-TDA) comprising thiophene as a strut. The structure analysis proved that the Co-TDA has 3D network structure with coordinated DMF molecules. Interestingly, cobalt ions form a unique cobalt-oxo 1D chain, which was further connected by thiophene dicarboxylate (TDA) to form a 3D network structure. Three independent cobalt ions were identified, 1) distorted octahedron geometry with one water molecule and TDA ligand, 2) octahedron with only TDA ligand and 3) square pyramidal with 2 DMF and TDA. The unique nature of cobalt structure allows us to study magnetic properties of the Co-TDA using superconducting quantum interference device (SQUID). Despite the non-porous nature of the framework, solvent removal may allow pore generation of the framework. Although the framework structure was slightly destructed by removal of solvent, re-exposure to the DMF allows regeneration of the original structure. Therefore, multiple open-metal coordination sites may be presented in the framework, which will be useful for strong gas binding. Using the desolvated framework, further gas sorption analysis is now in progress. Details of this work will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-115**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

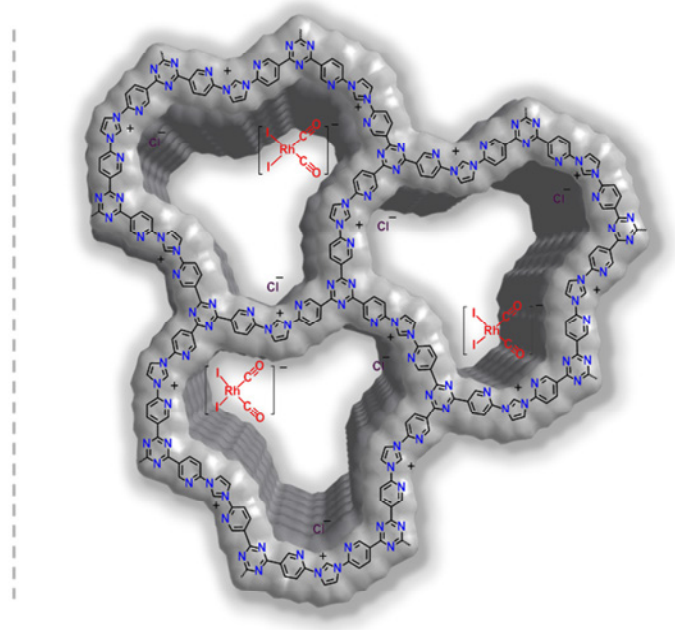
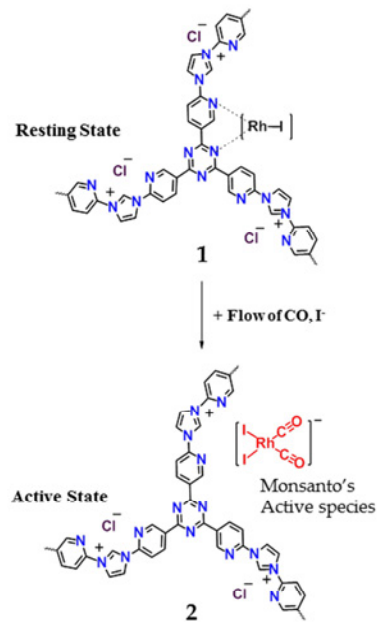
Heterogenization of Monsanto's catalyst on Covalent Triazine Framework functionalized with Imidazolium ionic structure; the efficient Methanol Carbonylation with Exceptional Stability

Kwangho Park, Seok-Chan KIM¹, Sungho Yoon^{*}

Department of Bionano Chemistry, Kookmin University, Korea

¹*Department of Chemistry, Kookmin University, Korea*

We present for the first time the synthesis and characterization of heterogenized Monsanto's Rh catalysts on charged 1,3-bis(pyridyl) imidazolium-based CTF (bpim-CTF) support for methanol carbonylation with the continuous plug-flow reaction in the gas phase. We found that the catalytic species was implemented as single site catalyst distributed through the support by the ligation to abundant N atom sites. Further, the catalytic activity was assessed through the effect of temperature, pressure, and reagents flow. The Rh-bpim-CTF catalyst featured higher efficiency than other heterogeneous catalytic systems, which may be attributed to the high electron donation from the N-rich environment of pore surface. Moreover, the long-term stability of the catalyst during the continuous process was confirmed without catalytic deactivation, derived by the ion-pair interaction between the positive-charged [imidazolium]⁺ moiety and Monsanto's active species (i.e. [Rh(CO)₂I₂]⁻).



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-116**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

TiO₂ modification with CuI for electron transport layer of Planar Perovskite Solar Cell

Taewan Kim, HONG IL KIM, Sangwon Kim, Taiho Park*

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

In planar TiO₂ perovskite solar cells, the low efficiency due to improper conduction band and low electron extraction ability was chronic problems. Herein, the planar TiO₂ electron transport layer for perovskite solar cells was modified by copper iodide (CuI) material with simple one step spin-coating process. The p-type nature of CuI islands on the TiO₂ surface shifted the band alignment of TiO₂, making barrier-free contact and increasing open circuit voltage. Furthermore, CuI on TiO₂ surface could pull the electron to the interface between perovskite and TiO₂, improving the electron extraction and reduced the non-radiative recombination. Consequently, the high efficiency (19.0%) planar-perovskite solar cell was fabricated. Interestingly, the hysteresis effect was almost eliminated, which was believed to be due to a removed trap sites by CuI.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: INOR.P-117

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facile Synthesis of N-doped Carbon Coated Zn₂SnO₄ Using Dopamine as an Anode Material for Lithium-Ion Batteries and Sodium-Ion Batteries

Namyeong Kim, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Zinc stannate (Zn₂SnO₄) is one of the attractive anode materials for lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs) because of its high discharge capacity of about 1231 mAh g⁻¹ in LIBs and 1004 mAh g⁻¹ in SIBs, respectively. However, Zn₂SnO₄ suffers from its large volume changes and severe particle aggregation during longer term cycles. These problems lead to particle pulverization, resulting in irreversible capacity and poor cycling stabilities. To overcome these problems, Zn₂SnO₄ was coated with N-doped carbon using dopamine as a carbon source in this study. Zn₂SnO₄ nanoparticles were successfully synthesized by a facile hydrothermal method. Subsequently, a layer of N-doped carbon is coated on Zn₂SnO₄ nanoparticles by ex situ methods using dopamine as carbon and nitrogen sources. The Zn₂SnO₄/N-doped carbon (Zn₂SnO₄/NC) composite shows the excellent cycling performance with the initial discharge capacities of about 1251 mAh g⁻¹ at 60 mA g⁻¹ in LIBs and 641 mAh g⁻¹ at 32 mA g⁻¹ in SIBs between 0.005 – 3.0 V. After 100 cycles, the discharge capacities of about 843 and 271 mAh g⁻¹ remained in LIBs and SIBs, correspondingly, revealing better capacity retention compared to bare Zn₂SnO₄.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-118**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Ruthenium Nitrosyl Complexes with modified salophen ligand

Minyoung Kim, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Nitric oxide plays important roles in a wide variety of physiological processes, including neurotransmission, immune response, blood pressure control, and inhibition of tumor growth. For the purpose of controlling the physiological processes, compounds that selectively release nitric oxide have attracted considerable interest. Among them, ruthenium nitrosyl complexes have been proposed as a photodynamic therapeutic agents in biomedicine and in tumor treatment. This research aims at developing ruthenium nitrosyl complexes which absorb long wavelength visible light to release NO and are dissolved in water. We present the strategies to develop visible-light sensitive NO-releasing Ru complexes with higher quantum yield. We introduced new ligands with hydroxyl group on the positions of ortho, meta and para of the salophen ligand in order to increase the solubility in water. In this study, we show the NO-releasing properties of the complexes monitored by UV-VIS, IR spectroscopy, EPR.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-119**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Visible-light-driven Photochemical CO₂ Reduction: Tuning and Optimization of Catalytic Performance of Dye/TiO₂/Mn(I) Ternary System

Sung-Jun Woo, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In photocatalytic systems for CO₂ reduction, Ru and Re complexes with 2,2'-bipyridine as ligand have been frequently investigated as catalysts. Although several systems with such catalysts showed selective CO₂ reduction with very high efficiency, however they include expensive rare metals. Mn is an earth abundant transition metal, and Mn is a same group with Re. In such, the metal complex containing manganese (Mn) metal can be considered as an alternative electrocatalyst for CO₂ reduction. In hybrid ternary system (Dye/TiO₂/electrocatalyst) for photolysis, the prepared bipyridyl Mn complex is used as an electrocatalyst for CO₂ reduction. The Mn complex-immobilized hybrid catalytic particles showed a high TNHCOOH of >250 during 30 h in a homemade merry-go-round type reactor (under LED lamp irradiation, $\lambda \geq 420$ nm).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-120**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

New insight into the non-conventional Porous Materials: Metal-Organic Triangles

Jiyeon Kim, Wonyoung Choe^{1,*}

Chemistry, Ulsan National Institute of Science and Technology, Korea

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

Designed porous materials have attracted great interest owing to their potential applications such as gas storage, separation and catalyst. Conventional porous materials are metal-organic frameworks (MOFs), metal-organic polyhedral (MOPs), and covalent-organic frameworks (COFs). However, UMOT (Metal-Organic Triangle) described in this presentation is a unique example of non-conventional porous material. The porous material with non-porous units has a great advantage. Because we can expect a possibility of featuring Bronsted acidic site using defect site of linker. UMOTs are synthesized by zirconium and TMBDC linkers (tetramethyl terephthalic acid). They show higher Qst value of 35.9 kJ/mol comparable to other MOPs or MOFs.

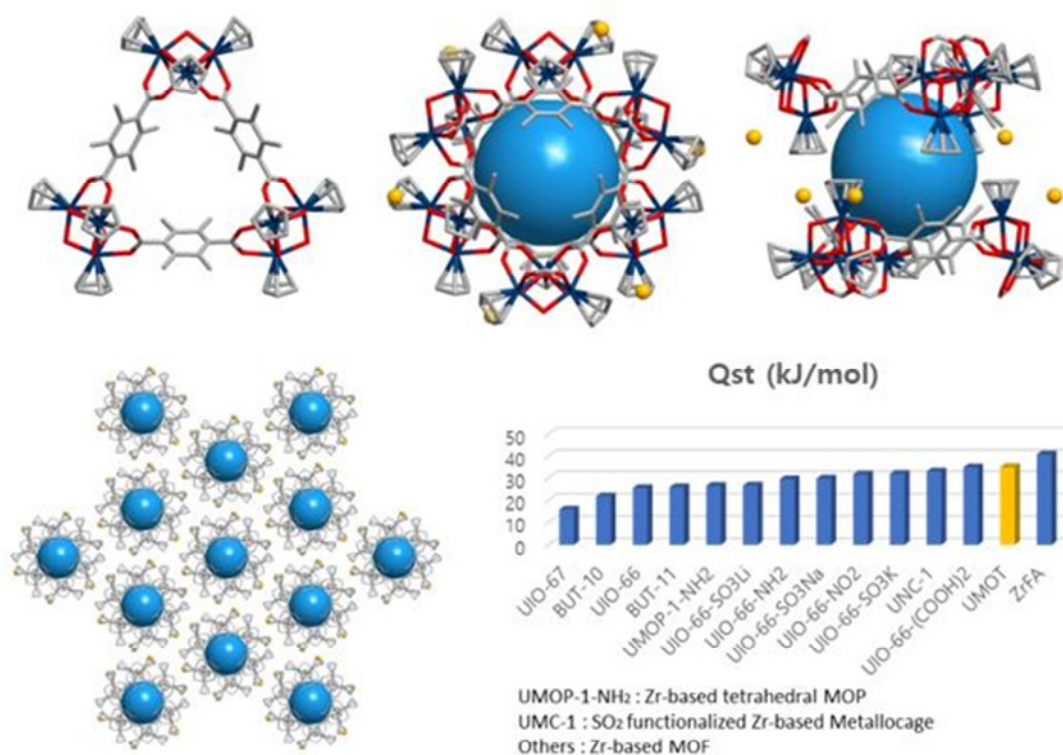


Figure 1. UMOT ($\{[Zr_3(\mu_3-O)(Cp)_3(\mu_2-OH)_3]_3(HCOO)_3(TMBDC)_3\}Cl_3$). Two UMOTs form a David star-shape dimer by C-H $\cdots\pi$ interaction. The dimers are packed in distorted FCC structure by hydrogen bonding. Qst graph of MOPs or MOFs.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-121**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly Efficient Photocatalytic CO₂-to-CO Conversion through new Hybrid binary System (Porphyrin Photosensitizer + TiO₂/ReC)

Seong-han Choi, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son *

Department of Advanced Materials Chemistry, Korea University, Korea

A series of zinc porphyrin complex (ZnPX-dY : (X = P;phenyl, D;2,6-Didodecylphenoxyphenyl), (Y = Si;Triisopropylsilyl, H;hydrogen) were applied as visible-light photosensitizer in solution to the selective CO₂ reduction to CO in the presence of an electron donor (BIH) and a hybrid catalyst (TiO₂/ReC) prepared by anchoring of Re(4,4'-Y₂-bpy)(CO)₃Cl (Y = CH₂PO(OH)₂) on TiO₂ particles. Irradiation of the system in *N,N*-dimethylformamide (DMF) at >500 nm resulted in the successful reduction of CO₂ to CO with efficiencies in the order X ZnPD-dH > ZnPP-dH > ZnPD-dSi > ZnPP-dSi. The systems undergo reactions during photocatalysis: hydrogenation of the porphyrin to form chlorin and isobacteriochlorin units is detected by visible absorption spectroscopy. The studies of sensitizers using mass spectroscopy also can provide insight into methods of activating CO₂. Mass spectroscopy analysis revealed that ZnPD-dSi was degraded to ZnPD-dH. However, it was further observed that porphyrin was decomposed into chlorin.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-122

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

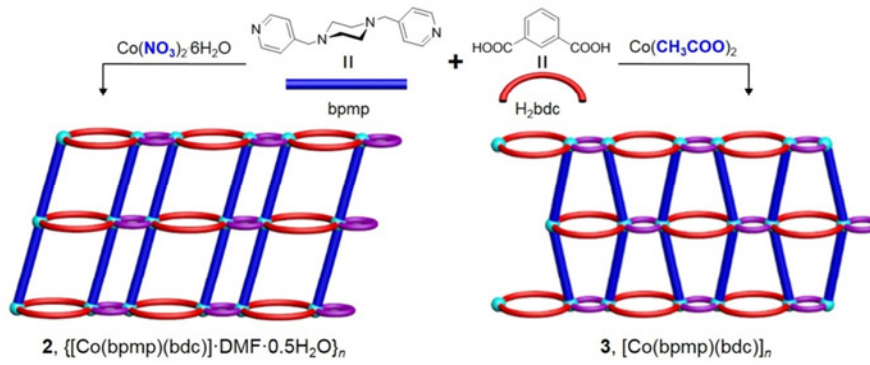
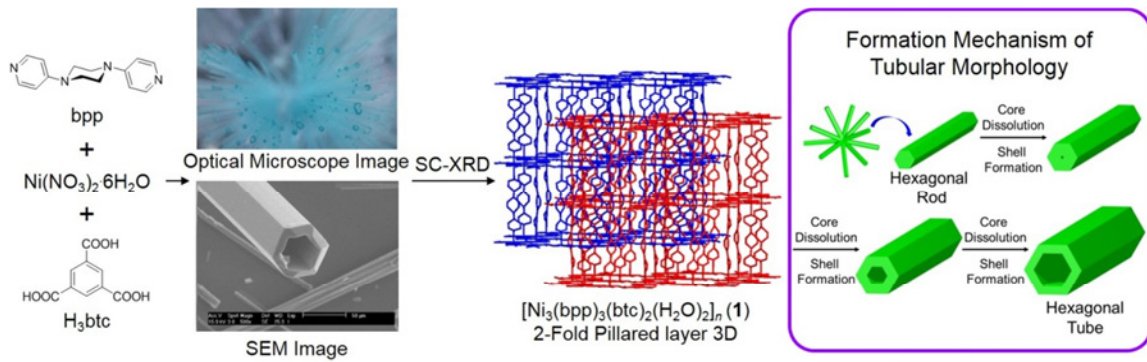
MOFs Based on Dipyridyl Piperazine and Benzene Carboxylate: Hexagonal Tubular Crystals of Ni(II) MOF and Anion-Dependent Co(II) MOFs

Huiyeong Ju, Eunji Lee, Leonard F. Lindoy^{1,*}, Shim Sung Lee^{*}

Department of Chemistry, Gyeongsang National University, Korea

¹*Department of Chemistry, The University of Sydney, Korea*

Binary ligand system of dipyridyl piperazine ligands (bpp and bpmp) and benzene carboxylic acids (H₃btc and H₂bdc) was employed to prepare MOFs. Interestingly, the solvothermal reaction of Ni(II), bpp, and H₃btc resulted in the formation of hexagonal tubular crystals which were identified as a double-interpenetrated 3D MOF, [Ni₃(bpp)₃(btc)₂(H₂O)₂]_n (**1**). The formation mechanism of the tubular morphology was proposed. While reactions of bpmp with Co(NO₃)₂·6H₂O and Co(CH₃COO)₂ in the presence of H₂bdc afforded 2D coordination polymers, {[Co(bpmp)(bdc)]·DMF·0.5H₂O}_n (**2**) and [Co(bpmp)(bdc)]_n (**3**), respectively. The 2D networks of **2** and **3** show different connectivity due to the conformational difference of the flexible bpmp linker ligand.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-123**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Polymetallic Catalysts bearing asymmetric tripodal ligand for CO₂ conversions

inyong lee, Jungseok Heo*

Department of Chemistry, Chungnam National University, Korea

For few decades, carbon dioxide has been considered one of the main causes leading to the greenhouse effect. Because of this concern, many scientists have researched a variety of applications utilizing carbon dioxide as a kind of sustainable resources. Among the applications, a cycloaddition reaction of CO₂ and epoxides to form useful cyclic carbonates is one of promising researches. For this application, we prepared a Schiff base type of ligand as a catalyst precursor by coupling 2,4,6-triformylphenol and 2-aminophenol. The precursor was successfully characterized by ¹H-NMR spectroscopy and single-crystal X-ray diffraction crystallography. The ligand was designed to possess three catalytic sites upon reaction with metal complexes. We investigated catalytic activity of its metal complex with several epoxides. Catalytic reactions under systematic reaction conditions were investigated and the details will be presented in the poster presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-124

Area: Inorganic Chemistry

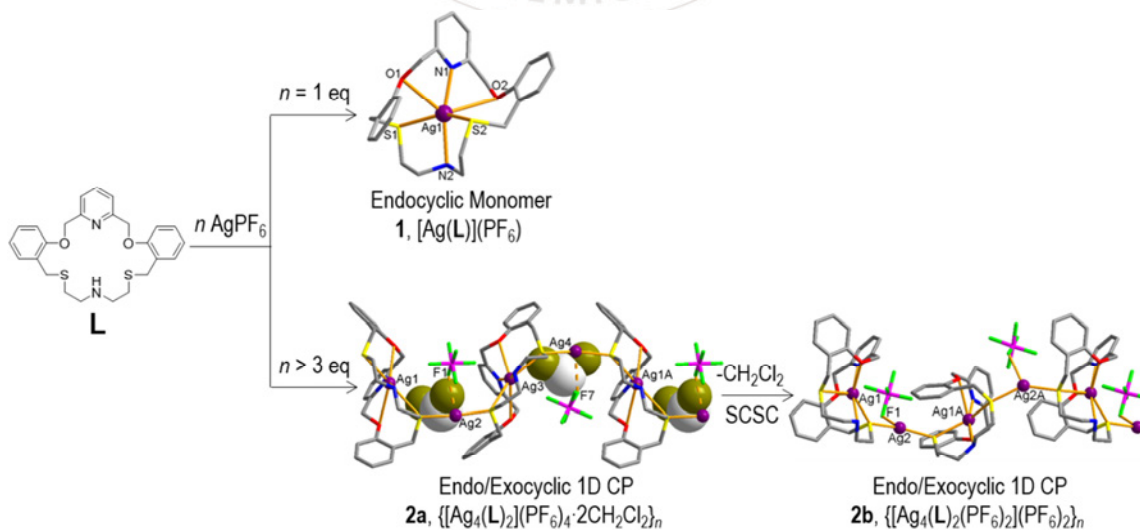
Type: Poster Presentation, Time: THU 11:00~12:30

Endo/Exocyclic 1-D Silver(I) Coordination Polymers with an N₂O₂S₂-Macrocycle Exhibiting Desolvation-Induced SCSC Transformation

Sujin Seo, Eunji Lee , Shim Sung Lee *

Department of Chemistry, Gyeongsang National University, Korea

An N₂O₂S₂-macrocycle (**L**)¹⁻³ incorporating one pyridine and two benzo subunit was employed and its silver(I) complexes are reported. Reaction of **L** with one equivalent AgPF₆ afforded a typical endocyclic 1:1 complex [Ag(**L**)](PF₆) (**1**). While, the use of three equivalents or above amount of AgPF₆ gave an endo/exocyclic 1-D coordination polymer {[Ag₄(**L**)₂](PF₆)₄·2CH₂Cl₂]_n (**2a**), in which the endocyclic complex units are linked by the -^{endo}Ag-S-^{exo}Ag-S- bond to form an infinite chain. In addition, when single crystals of **2a** was undisturbed in air, the lattice solvent molecules were removed to give a desolvated {[Ag₄(**L**)₂](PF₆)₂](PF₆)₂]_n (**2b**) which accompanies the conversion of the coordination environments in a single-crystal to single-crystal (SCSC) manner.



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Code: INOR.P-125

Area: Inorganic Chemistry

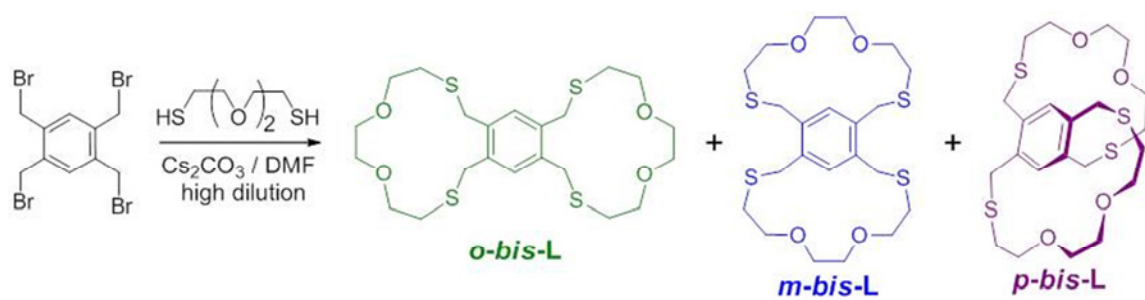
Type: Poster Presentation, Time: THU 11:00~12:30

Crystal Engineering of Bis-O₂S₂-Macrocyclic Isomers: Isolation of para-Isomer as Final Puzzle, and Borderline and Soft Metal Complexes

Seulgi Kim, Shim Sung Lee*

Department of Chemistry, Gyeongsang National University, Korea

In addition to *ortho*-form (***o*-bis-L**) and *meta*-form (***m*-bis-L**) of bis-O₂S₂-macrocyclic regioisomers obtained previously^{1,2}, the *para*-form (***p*-bis-L**) was newly isolated and the three completed isomers were structurally characterized by single crystal X-ray analysis.³ In complexations, borderline (Pb²⁺) and soft (Hg²⁺ and Cu⁺) metal salts were employed to investigate the isomer effect on the coordination modes and topologies of the resulting supramolecular coordination products. The lead(II) perchlorate afforded an infinite one-dimensional (1-D) coordination polymer {[Pb₂(***o*-bis-L**)(μ-ClO₄)₂(ClO₄)₂]}_n (**1**) and a discrete complex [Pb₂(***m*-bis-L**)(CH₃CN)₂(H₂O)₂(ClO₄)₂](ClO₄)₂ (**2**), both of which are based on the endocyclic binuclear complexes mainly due to the oxophilicity of lead(II) ion. Meanwhile, mercury(II) halides showed an exocyclic dinuclear complex [Hg₂(***o*-bis-L**)I₂][Hg₃I₈] (**3**) and an exocyclic 1-D coordination polymer [Hg₃(***m*-bis-L**)Br₆]_n (**4**) because the differences of sulfur-to-sulfur separation in the free ligand isomers might induce the discriminated coordination modes. When a mixture of mercury(II) iodide and copper(I) iodide was used in the reaction with ***m*-bis-L**, a heterometallic 1-D coordination polymer [Cu₂Hg₂I₄(***m*-bis-L**)(μ-Cu₂I₄)(CH₃CN)₂]_n (**5**) was obtained. In **5**, the exocyclic dicopper(I) complex units are linked by -Hg-Cu₂I₄-Hg- segments to form a zigzag chain. Consequently, unlike the borderline metal, the soft metal ion shows the sulfur-to-sulfur separation dependent coordination modes. The present study demonstrates how small differences in the structural isomerism of ligands impact their self-assembled coordination products in terms of coordination modes, topological structures, and physicochemical properties. **References**[1] Siewe, A. D.; Kim, J.-Y.; Kim, S.; Park, I.-H.; Lee, S. S. *Inorg. Chem.* **2014**, *53*, 393.[2] Kim, S.; Siewe, A. D.; Lee, E.; Ju, H.; Park, I.-H.; Park, K.-M.; Ikeda, M.; Habata, Y.; Lee, S. S. *Inorg. Chem.* **2016**, *55*, 2018.[3] Kim, S.; Lee, S. S. Manuscript is in preparing for publication.



Conference Date: October 18~20, 2017

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Code: **INOR.P-126**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solar H₂ Evolution in Water with Red-Light-Absorbing Hybrid Ternary System (Squaraine dye/TiO₂/Pt)

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Department of Advanced Materials Chemistry, Korea University, Korea

Using solar energy to split water for the production of renewable hydrogen (H₂) is a promising strategy to satisfy our demand for sustainable and storable energy. For light-to-chemical energy conversion, the photochemical splitting of water into hydrogen and oxygen is a key issue in artificial photosynthesis. Dye-sensitized photocatalysis has emerged as a functional bio-inspired approach for sunlight-driven H₂ evolution in water by means of co-immobilising a dye and a catalyst on semiconductor in suspension. As a role model, natural photosystem has only used the limited region (red light) among visible light for light-harvesting with efficient blue light protection by carotenoids (as carotenoids absorb blue light), functioning as photoprotectants in photosynthesis. Therefore, low-energy photo-sensitization is a key issue in the realization of solar light harvesting for highly efficient artificial photosynthesis systems and solar cells. The introduction of efficient red light absorption dye is very essential (desirable) to build an efficient artificial photosynthetic system with obtaining its long-term durability. Squaraine dyes are one of the most promising candidates owing to their high extinction coefficients in NIR region (600-800 nm) and easy synthetic route. Herein, we present the detailed characterization and principles of hybrid system (Dye/TiO₂/Pt) for H₂ evolution, which is constructed by the anchoring of both red light active squaraine (sensitizer) and Platinum on metal oxide particles. This study includes some interesting findings from the structural modification of squaraine sensitizer and the spectral range control of irradiated light source that influence the long-term stability of overall photocatalytic system.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-127**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A trihydroxyphenol-appended benzene-1,3,5-tricarboxamide-involved electrospun film for chromogenic detection and removal of Cs⁺

Na Young Lim, Junho Ahn, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Cesium is a common contaminant in industrial, medical and nuclear wastes, and can cause several health problems. Therefore, the development of chemical probes and adsorbents for cesium is important. tri- or dihydroxyphenyl-appended BTAs 1 and 2 were synthesized and their chromogenic sensing properties were studied. Interestingly, ligands 1 and 2 formed fibrous structures with ca. 50–100 nm diameters in aqueous solution and spherical structures with 100–200 nm diameters in the presence of Cs⁺. The colorless self-assembled ligands 1 and 2 changed to yellow in the presence of Cs⁺ owing mainly to the cation- π interaction as well as π - π stacking. In contrast, no significant color changes in 1 and 2 were observed upon addition of other metal ions. A film incorporating 1 was prepared by the electrospinning method. This film showed a selective color change in Cs⁺. The detection limit of the film for cesium was higher than that for a bulk solution of 1, which can be ascribed to its larger surface area. Thus, adsorption percent of EF-1 for Cs⁺ was increased by film size. EF-1 was able to remove Cs⁺ up to 100 ppb. concentration of EF-1. this method is potentially useful for the detection of cesium contamination caused by the nuclear industry, waste water, and biological systems. Therefore, EF-1 shows promise as a portable sensor for the detection of Cs⁺ in aqueous solution.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-128**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Mesoporous silica-Au nanoparticle-based mitochondria-targeting drug delivery system of doxorubicin and F16

Junho Ahn, Hee Kyoung Choi, Ka Young Kim, Jong Hwa Jung *

Department of Chemistry, Gyeongsang National University, Korea

We fabricated mitochondria-targetable doxorubicin-loaded mesoporous silica (DOX-FITC/Py-MSN) decorated with folate/F16-carboxylpillar[5]arene-capped Au nanoparticles (CP-AuNPs). Pyridinium derivative and Fluorescein isothiocyanate isomer I (FITC)-modified mesoporous silica were fabricated by sol-gel polymerizations of alkoxy silane groups. Doxorubicin was loaded into the FITC/Py-MSN and quantification of loaded doxorubicin in FITC/Py-MSN was used by UV-Vis measurements. CP-AuNPs were formed by NaBH₄-utilized reduction of Au³⁺ containing CP were self-assembled with pyridinium groups involved in FITC/Py-MSN, Folate, F16 respectively. Self-assembled nanoparticles (NP-1) of doxorubicin-loaded FITC/Py-MSN (NP-2) and Folate/F16-loaded CP-AuNPs induced by interaction of pillar[5]arene and pyridinium derivatives were confirmed by TEM, IR, UV-Vis, zeta potential analysis. To demonstrate mitochondria-targeting of NP-2 in cancer cells, we measured confocal laser scanning microscopy. Co-localizations of doxorubicin, FITC, mito-tracker in mitochondria was observed within 2 hours. FITC/Py-MSN had cytotoxicity on HeLa cells when a hundred milligram of FITC/Py-MSN were treated. Anticancer effect of Doxorubicin was confirmed. NP-1 consisted of Folate/F16-loaded CP-AuNPs and DOX-FITC/Py-MSN were successfully penetrate cancer cells and had synergistic cytotoxic effect on cancer cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-129**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Helical Self-Assembly and Luminescent Properties of Alkynylplatinum(II) Terpyridine Complexes of C_3 Space Group

Jaehyeon Park, Ka Young Kim, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Alkynylplatinum(II) terpyridine complexes containing the Triphenylamine (TPA) as core group was synthesized. Helical fibrous nanostructures were obtained through supramolecular assembly with the platinum(II) acetylene complexes via intermolecular hydrogen bonding, amphiphilic effects, Pt···Pt interactions, and π - π stacking interactions. Helical fibrous exhibited the strong luminescence, which was dependent to the solvent polarity in this conference, we will present on the preparation of alkynylplatinum(II) Terpyridine complex and its spectroscopic property. The induced complex self-assembly and luminescent were found to be influenced by the solvent polarity. Through UV/Vis absorption, emission, circular dichroism, and ^1H NMR studies, the contribution of hydrogen bonding, Pt···Pt and π - π stacking interactions as driving forces for Helical self-assembly have been established.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-130

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Selective and efficient Photocatalytic CO₂-to-CO conversion by New Hybrid system consisting of bis-cyclometalated bipyridyl Ir(III) photosensitizer and Re(I)-complex-anchored TiO₂ catalytic particles

Hayeon Cheong, So-Yoen Kim, Yang-Jin Cho, DAE WON CHO, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Five cyclometalated cationic iridium complexes ($[\text{Ir}(\text{btp})_2(\text{bpy}-\text{X}_2)]^+$ ($\text{Ir}-\text{X}^+$: btp = (2-pyridyl)benzo[*b*]thiophen-3-yl; $\text{bpy}-\text{X}_2$ = 4,4'- X_2 -2,2'-bipyridine (X = OMe, ^tBu, Me, H, and CN)) were prepared as visible-light photosensitizer. CO-producing Re(I) catalyst on TiO₂ produced CO (selective) in CO₂-saturated DMF/water solution containing 0.1 M BIH (electron donor) and 1 mM photosensitizer. Irradiation of the system at >400 nm resulted in the successful reduction of CO₂ to CO with efficiencies in the order $\text{X} = \text{}^t\text{Bu} \sim \text{Me} > \text{OMe} > \text{H}$; $\text{Ir}-\text{CN}^+$ has no photosensitization effect. An interesting observation is that $\text{Ir}-\text{}^t\text{Bu}^+$ and $\text{Ir}-\text{Me}^+$ are less efficient than $\text{Ir}-\text{OMe}^+$ at an early stage of the reaction but reveal persistent photosensitization behavior for a longer period of time unlike the latter. The persistent photosensitization behavior of $\text{Ir}-\text{}^t\text{Bu}^+$ should arise from the photochemical stability of $[\text{Ir}-\text{}^t\text{Bu}^+]^*$ while the photochemical labile property of $[\text{Ir}-\text{OMe}^+]^*$ leads to the levelling-off behavior in the photosensitized CO₂ reduction. Implications of the present observations and reaction mechanisms are discussed in detail.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-131**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Transfer and Inversion of Co-assembled Supramolecular Chirality in Hydrogel: Transformation of 2D-Sheet to Rolled-Up Tubular Structure

Heekyoung Choi, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We have demonstrated transfer and inversion of supramolecular chirality from chiral calix[4]arene analogues (**2D** and **2L**) having alanine moiety to achiral bipyridine derivative (**1**) having glycine moieties in co-assembled hydrogel. Molecular chirality of **2D** and **2L** could transfer supramolecular chirality to an achiral bipyridine derivative **1**. Moreover, upon addition of 0.6 equivalent of **2D** or **2L** to **1** induced the supramolecular chirality inversion of **1**. More interestingly, 2D-sheet structure of co-assembled hydrogels formed with 0.2 equivalent of **2D** or **2L** was changed to roll up into tubular structure in the presence of 0.6 equivalent of **2D** or **2L**. The chirality inversion and morphology change is mainly mediated by intermolecular hydrogen bonding interactions between the achiral and chiral molecules, which might be induced reorientations for the assembled molecules, as confirmed by density functional theory (DFT) calculations.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-132**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation of Color-Tunable Fluorescent Multiblock Complexes

Ka Young Kim, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

The significant contribution of conventional living polymerization to polymer science assures that living supramolecular polymerization will lead to a variety of novel phenomena and applications. To achieve this, self-organization occurring far from thermodynamic equilibrium-ubiquitously observed in nature must take place. Prion infection is one example that can be observed in biological systems. We have investigated the assembly phenomenon using isodesmic and cooperative models and found that it occurs through a delicate interplay of these two aggregation pathways. Here, we will present on 'artificial infection' process in which benzene-1,3,5-tricarboxamide-based monomers complexes with metal ions assemble into nanoparticles, and the nanoparticles are then converted into nanofibres in the presence of an aliquot of the nanofibre or a lot of metal ion.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-133**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nickel(II) Ions-Switchable Helicity of Bipyridine-Based Polymergel

Misun Go, Heekyoung Choi, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We demonstrated different origins of helical directions of polymeric gels derived from hydrazine reaction in the absence and the presence of Ni²⁺. The right-handed helicity of polymeric gel without Ni²⁺ originated from the stereoenantiomeric D-form alanine moiety embedded in the building block. In contrast, the right-handed helicity was inverted to the left-handed helical direction upon addition of Ni²⁺, indicative no influence to stereoenantiomer embedded in the building block in the supramolecular level. More interestingly, we could finely control the distribution of the right- to the left-handed helical fibers by adjusting concentrations of Ni²⁺, which converted from 100% of the right-handed helical fiber to 70% of the left-handed helical fiber. In the presence of Ni²⁺, both the right- and the left-handed helical fibers co-existed in the supramolecular level. Some fibers also revealed both the right- and left-handed helical directions in single fiber.

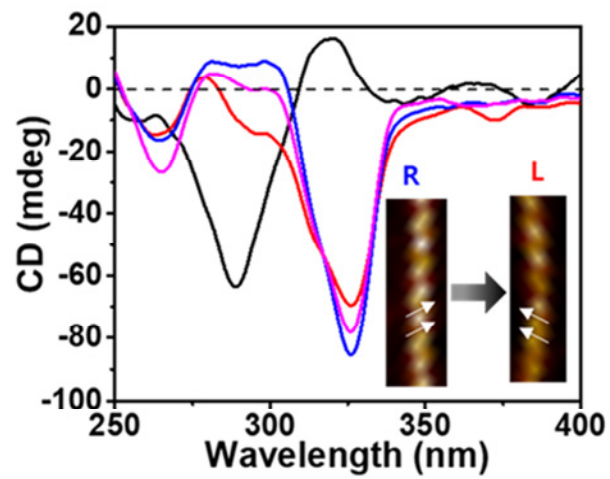


Figure 1. (A) Circular dichroism spectra and atomic force microscopy images.



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Code: **INOR.P-134**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

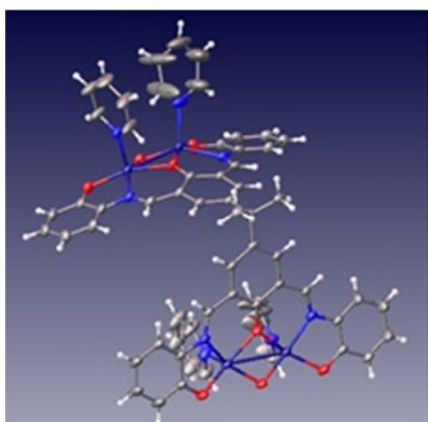
Bent shape of Bis-bimetallic Zn-catalyst for Cycloadditions of CO₂ to epoxides

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

Not only as solutions for CO₂ emission issue, but also as promising CCU technologies, chemical reactions producing cyclic carbonate and polycarbonate are attracting great attentions from both academic researchers and industries. [1-3] For practical applications, the whole R&D is focused onto finding and optimizations catalysts to make it efficient and cost-competitive. We present a new Zn-catalyst in which two bimetallic centers are connected via a sp³ carbon taking bent shape of overall geometry. In the crystal structure, Zn to Zn distance in a bimetallic centers is 3.126 Å and distance between bimetallic centers is 11.036 Å. The overall structure of the catalyst was designed to maximize cooperative effects among attached substrates during the catalytic process. In the poster session, test reaction results under various conditions will be discussed.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-135

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Helix to Super Helix Transition in Co-Assembly Based C_3 Symmetric Molecular

Hyowon Seo, Heekyoung Choi, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We prepared building blocks **1** and **2** to fabricate supramolecular co-assembly. The supramolecular helicity of co-assembly was characterized by circular dichroism (CD) and atomic force microscope (AFM). The co-assembly exhibited well-organized helical fiber structure by AFM image. In particular, upon addition of **2** in co-assembly induced dramatic CD enhancement. In this conference, we will present super helix of co-assembly.

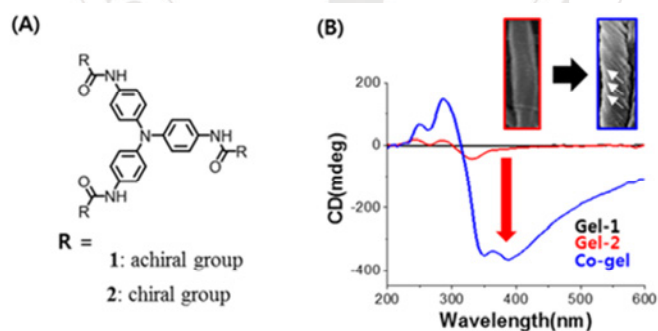


Figure 1. (A) Chemical structures of **1** and **2**. (B) Circular dichroism (CD) spectra and scanning electron microscope microscopy (SEM) images.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-136

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Zn-MOFs Containing Flexible Dicarboxylates with 1,2-Bis(4-pyridyl)ethane or 1,2-Bis(4-pyridyl)ethylene Ligands

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

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Six flexible α,ω -alkane-(or alkene)-dicarboxylates (mal(1), suc(2), fum(3), glu(4), adi(5), and muc(6)) produced 3-D or 2-D Zn^{II} frameworks with bpa or bpe pillars. For bpa pillar system, 3-D frameworks of 2-bpa, 3-bpa, 5-bpa, and 6-bpa formulated as $[\text{Zn}(\mu_2\text{-O}_2\text{CRCO}_2)(\mu_2\text{-bpa})]$ containing water solvates show 4-fold or 5-fold interpenetrated, uninodal, 4-connected dia networks with a tetrahedral geometry around a Zn^{II} ion. 1-bpa and 4-bpa formulated as $[\{\text{Zn}(\text{H}_2\text{O})(\text{O}_2\text{CRCO}_2)\}_2(\mu\text{-bpa})]$ contain coordinated water ligands with different structures. For bpe pillar system, 3-D frameworks of 3-bpe and 6-bpe formulated as $[\text{Zn}(\mu_2\text{-O}_2\text{CRCO}_2)(\mu_2\text{-bpe})]$ with water and DMF (or DEF) solvates show 3-fold or 4-fold interpenetrated, unimodal, 4-connected dia networks with a distorted tetrahedral coordination geometry around a Zn^{II} ion. 1-bpe shows a 3-D framework formulated as $[\{\text{Zn}(\text{H}_2\text{O})(\mu_2\text{-mal})\}_2(\mu_2\text{-bpe})]$ with octahedral geometry around a Zn^{II} ion, and 4-bpe formulated as $[\text{Zn}(\mu_2\text{-glu})(\mu_2\text{-bpe})]\cdot 2\text{H}_2\text{O}$ shows a 2-D layer compound with a tetrahedral geometry around a Zn^{II} ion from two glu oxygen atoms and two bpe nitrogen atoms. 2-bpe formulated as $[\text{Zn}_2(\mu_4\text{-suc})(\mu_3\text{-suc})(\mu_2\text{-bpe})]$ shows a 2-D layer compound containing two asymmetric Zn^{II} ions with penta-coordinate and octahedral geometries. 5-bpe with the $[\text{Zn}(\mu_4\text{-adi})_{0.5}(\mu_2\text{-adi})_{0.5}(\mu_2\text{-bpe})]\cdot (\text{H}_2\text{O})$ formula contains two adipate types; one adi bridges four Zn^{II} ions and the other adi bridges two Zn^{II} ions with a chelating mode for each carboxylate. The results from bpa and bpe systems with the same dicarboxylate series support the same conclusion that there is a deep relationship between the structural dimensions and the coordination geometry/coordination modes of dicarboxylates. Most of all, the 3-D diamond-like structures should have a tetrahedral coordination geometry around Zn^{II} ions and monodentate coordination modes of carboxylates are preferred.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-137**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

O₂ activation from a bulky iron amino triphenolate complex

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Dioxygen activation with well-defined first-row transition metal complexes has been of great interests due to their potential application to aerobic oxidation of organic substrates, inspired by various enzymes to functionalize diverse substrates highly selectively utilizing oxygen. Although various well-defined iron complexes have been intensively investigated for the reactivity with O₂, dioxygen activation with high-valent iron complexes supported with phenolate ligands has less been studied. We designed a new iron(II) amino triphenolate complex with a high steric demand for activation of dioxygen and subsequent cleavage of dioxygen bond. Surprisingly, the progress was also characterized by single-crystal to single-crystal transformation upon exposure of dioxygen. Synthesis, characterization, and potential applications of the complexes will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-138**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Characterization and Fabrication of Mo Thin Film Coated on Soda Lime Glass for the CIGSeS Photovoltaic Application

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The molybdenum thin film (Mo-TF) was sputtered on soda lime glass (SLG) substrate using direct current (DC) magnetron sputtering system via different DC voltage. Their structural and adhesive, optical, electrical and mechanical properties were examined with respect to the deposition time and power. The peak intensity of XRD is maximized when DC sputter voltage is higher though planar resistance is under $1 \Omega/\square$. Also, the basic property of Mo-TF layer was measured by 4-point probe, AFM, SEM and UV-visible spectroscopy. We optimized the filming conditions of Mo-TF layer for the use of bottom electrode of CIGSeS photovoltaic (PV) cells by analyzing the effect of electrical and optical properties of Mo electrodes on the power conversion efficiency of CIGSeS PV cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-139**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fabrication of Inorganic CsPbX₃(X=Br, I) Perovskite Quantum Dot-based Remote-type White Down-Converted LEDs

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¹*Department of Bionano Chemistry, Kookmin University, Korea*

In this study, we synthesized all Inorganic perovskite (CsPbX₃(X=Br, I)) quantum dots (QDs) and fabricated remote type white DC-LEDs. CsPbX₃ perovskite QDs were synthesized using colloidal hot injection method and emission wavelength can be tuned 490 nm to 640 nm. CsPbX₃ QDs show the quantum yield from 50% to 85% and full-width at half-maximum (FWHM) range from 20 nm to 50 nm. CsPbX₃ inorganic perovskite QD-based remote-type DC-LEDs were fabricated combining perovskite QDs and InGaN blue (B) LED chip. We fabricated multi-layer white DC-LEDs using GR colored CsPbX₃ QD films covered on an InGaN-based B-LED. The optical properties of synthesized CsPbX₃ QDs were measured by photoluminescence (PL), UV-Vis spectroscopy and their structural properties were measured by X-ray diffraction (XRD), transmission electron microscopy (TEM). Fabricated monochromatic DC-LEDs were measured by electroluminescence (EL) spectrophotometer in the applied current range between 10 to 120 mA.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-140**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Realization of Display Backlight using Green and Red InP/ZnSeS/ZnS Multilayered Films

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To fabricate the QD down-converted white-LED (DC-WLED) backlighting systems of LCD displays, we synthesized green and red (GR)-emitting InP/ZnSeS/ZnS quantum dots (QDs) and fabricated green and red multi-layered QD films. The GR emissive InP/ZnSeS/ZnS QDs were synthesized using a colloidal hot injection method. The dominant wavelength of GR color of QDs are 519nm and 599nm, respectively and the quantum yields of both G and R InP-based QDs are approaching to ~75%. The full-width at half maximum (FWHM) values of both GR InP-based QDs are 50nm and 63nm, respectively. We fabricated the GR InP/ZnSeS/ZnS multi-layered thin-films with UV curable binder, and realized the LCD backlighting system with InGaN blue LED chip. Finally, we measured the optical properties of DC-WLEDs incorporated with GR InP-based QDs, such as luminous efficacy (LE), correlated color temperature (CCT), and the color coordinates using an electroluminescence (EL) spectrophotometer.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-141**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Red Shift of Photoluminescence Excitation Spectra of Narrowband BaMgAl₁₀O₁₇:Eu,Mn Green Phosphors

HEEJOON KANG, KEYONG LEE, Ji Hye Oh, YOUNG RAG DO*

Department of Bionano Chemistry, Kookmin University, Korea

Vacuum ultraviolet (VUV) phosphors are not used in recent display market because PDP displays were terminated several years ago by low device efficiency and resolution limit. However, one of PDP phosphors can be used in the light-emitting diodes, owing to the high stability and wide band gap of host materials. Here, we introduced the challenge to use BaMgAl₁₀O₁₇:Eu,Mn (BAM:Eu,Mn) phosphors to be used in narrow-band LED green phosphors for backlighting use. To satisfy the requirements of BAM:Eu,Mn phosphors for LED application, the photoluminescence excitation (PLE) spectrum of the BAM:Eu,Mn phosphor should be moved from the violet to deep blue (431~435 nm) by substituting Ba²⁺ with Sr²⁺, Eu²⁺, or Ca²⁺ ions. They also should maximize the energy transfer from the absorbed blue energy of Eu²⁺ to the Mn²⁺ ions by optimizing the concentrations of both Eu²⁺ and Mn²⁺ ions. Finally, the PL emission of the narrowband 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 analyzed and discussed the optimum conditions of synthesizing blue-excited green phosphors and the possibility of their application into phosphor-converted white LEDs.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: INOR.P-142

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fabrication of Metal-Insulator-Metal Structure (ITO-Al₂O₃-Ti/Au) to evaluate breakdown voltage of ALD-coated Al₂O₃ Thin Films

**Young Kwon Jang, Gang-Yeoul Ryu¹, HEEJOON KANG², YunJae Eo³, Woong Kim⁴,
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In this study, we fabricated the metal-insulator-metal (M-I-M) split structure using ITO-Al₂O₃-Ti/Au in microscale and measured the breakdown voltage of nano-thickness Al₂O₃ films deposited by atomic layer deposition (ALD) method. We developed M-I-M split structure to prevent the electrical short passages between top and bottom electrode of conventional vertically deposited M-I-M structure. First, we patterned ITO layer using photolithography and deposited nano-thick Al₂O₃ by ALD with various thickness (10, 20, 30, 40, 50 nm) at 200 °C. After then, we deposited Ti/Au metal (100 nm) using e-beam evaporator on the ITO/Al₂O₃ layer. Finally, we measured I-V curve from -10 V to 10 V using probe station. In addition, we analyzed the electrical, optical, morphological and structural properties of various nano-thick Al₂O₃ films. As a result, we successfully fabricated split M-I-M structure which couldn't have electronic short problem for optimizing insulating properties of ALD deposited Al₂O₃ films.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **INOR.P-143**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Coumaraz-2-on-4-ylidene: The Most π -acidic *N*-heterocyclic Carbene

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

¹*Pohang University of Science and Technology, Korea*

Recently, *N*-heterocyclic carbenes (NHCs) have attracted much attention as ligands that can effectively stabilize electron-rich unstable transition metal complexes and main-group elements. In addition, there are numerous studies on the activations of various chemical bonds based on the high reactivity of NHCs. These studies suggest that the reactivity of NHCs is strongly influenced by their HOMO-LUMO energy gap and singlet-triplet transition energy. To access NHC with the smallest energy gaps, we designed new NHCs called 'coumaraz-2-on-4-ylidene'. The various precursors of coumaraz-2-on-4-ylidene were successfully synthesized by simple two steps. The synthesis of their transition metal complexes and the specific reactivity of the NHCs were confirmed by in-situ generation and complexation from the precursors. Interestingly, the ⁷⁷Se chemical shift of the selenium adducts show that the coumaraz-2-on-4-ylidene has the lowest LUMO energy level compared with other NHCs. Additionally, we successfully tuned the electronic structure of coumaraz-2-on-4-ylidene using various functional group.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-144**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

[C₆H₅CH₂NH₃]₃BiCl₆·0.5H₂O: Photoluminescence Properties of a Red-emitting One-dimensional Organic Bismuth Halide

Seung-Jin Oh, TaeHwan Moon, JIYOON HWANG, Hyeshin Lee, Kang Min Ok*

Department of Chemistry, Chung-Ang University, Korea

A novel red-emitting one-dimensional organic-inorganic hybrid, [C₆H₅CH₂NH₃]₃BiCl₆·0.5H₂O, has been synthesized by the slow evaporation method and characterized by single crystal X-ray diffraction using synchrotron at 100K. It crystallizes in the monoclinic space group, *P*2₁/*c*, in which the unit cell parameters are *a* = 17.044(3) Å, *b* = 7.6090(15) Å, *c* = 22.478(5) Å, and β = 102.31(3)°. The crystal consists of a corner sharing octahedral bismuth chloride chains [BiCl₆³⁻]_∞ along the *b*-axis, which are surrounded by the benzyl ammonium C₆H₅CH₂NH₃⁺, chloride, and lattice water between the chains. The chains are linked via hydrogen bonds and ionic interaction between Cl···H(OW) and N-H···Cl, respectively. This unique one-dimensional structure makes it possible to emit strong photoluminescence properties in red-light region at room temperature. The detailed characterization of its optical properties, such as photoluminescence spectra, Infrared spectra, and UV-vis reflectance spectra, are also investigated.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **INOR.P-145**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Organic Mixed-Valence Systems of Rigid, Cofacially Compressed Aromatic Units for the Evaluation of Electron and Hole Transfer through π -Stacked Manifold

Hae Won Jung, Do Hoon Jun, Youn Kyung Kang*

Department of Chemistry, Sangmyung University, Korea

Electronic couplings mediated by series π -stacked aromatic components were evaluated with organic mixed-valence systems. Precursor molecules for the cation radical systems (DND, DNPND, and DNPND) and anion radical systems (QNQ, QNPNQ, QNPND) where D = 2,5-dimethoxybenzene electron donor component, N = 1,8-naphthyl pillaring motif, P = 1,4-phenylene spacer, and Q = 2,5-diene-1,4-dione electron acceptor component were synthesized via Pd-catalyzed cross-coupling reactions. Geometrical structure of DNPND was determined by X-ray crystallography while those of the rest were obtained by DFT calculations. Such structures manifest sub van der Waals interplanar separations between juxtaposed D (or Q) and P components enforced by 1,8-naphthyl group. Electrochemical experiments gave an insight that QNQ^{•-}, QNPNQ^{•-}, and QNPND^{•-} can be categorized as class III, II, and I of Robin & Day classification, respectively. Cation radical mixed-valence systems exhibited similar behavior. Further examination of optical transitions calculated by TD-DFT method provided quantitative electronic coupling values of these series based on Mulliken-Hush analysis within the weak coupling limit, which are in good agreement with electrochemical experiments.

Conference Date: October 18~20, 2017

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Code: **INOR.P-146**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Detail status of BL2D-Supramolecular Crystallography Beamline at the Pohang Accelerator Laboratory

Dae-Woong Kim, Dohyun Moon *

Beam Operation Team, Pohang Accelerator Laboratory, Korea

Supramolecular Crystallography Beamline (BL2D-SMC) at the Pohang Accelerator Laboratory is the unique crystallography beamline using synchrotron radiation in Korea. This beamline is suitable for experiment of small and supra molecule single crystal. The crystallography is a useful technique for determining the atomic and molecular structure of a crystal. It should be required fine and high-flux X-ray for generate good structure solution. Currently BL2D-SMC is supported high-flux X-ray with diverse wavelength range from 1.5 to 0.6 Å, and easy changeable temperature with 85 to 500K as a Cryojet 5 instrument. These devices can be easily used by user own through beamline software (BL2D-SMDC). The beamline will plan to change the high speed and durable large area CCD detector (Rayonix MX225HS) in this winter. This CCD is faster more than 10 times current installed ADSC Q210 CCD. It will give a chance to get the structural change of the single crystals. In this poster, we explain the BL2D beamline at Pohang Light Source II and to introduce the plan to change new CCD detector.

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Code: **INOR.P-147**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Crystallographic Evidence for Sensing of Nitroaromatic Compounds by MOF

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It highly desirable to detect the traces of explosives materials with the easy and cost effective manner for security, military issues and environmental protection. Trinitrophenol (TNP) has the higher explosive power amongst the nitro aromatic explosives even more than trinitrotoluene (TNT) and causes strong irritation and allergic reactions.(1) Plenty of works are reported using MOFs to selectively sense TNP featuring Lewis basic pyridyl or free amine sites inside the pores that are expected to induce electrostatic and hydrogen-bonding interactions. However, no direct evidence has been affirmed till date about the interaction of TNP molecule with MOF which leaves the sensing mechanism of TNP and the use of other functionality in ambiguity. We synthesized hydroxyl functionalized new MIL-53 analogous MOF using Indium nitrate and 2,5-dihydroxyterephthalic acid which shows high water stability and strong fluorescence at 450nm when excited at 352 nm. The MOF was used for sensing of nitroaromatic compounds (NAC) and shows very high selective quenching for TNP. The Stern Volmer constant (K_{sv}) value for TNP was calculated to be $8.8 \times 10^4 \text{ M}^{-1}$.(2) We further investigated the dynamics of quenching, performing fluorescence lifetime experiment which resulted in no change for fluorescence lifetime of MOF and suggests that static quenching is the major reason behind quenching of TNP. Crystal structure evidently reveals good pi-pi interaction of TNP with ligand moiety of framework and hydrogen bonding with MOF framework. This study provides new insight into the study of luminescence quenching mechanism for selective sensing of TNP suggesting that functionality capable of having hydrogen bonding interaction with TNP can be a successful candidate for selective sensing for TNP.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: INOR.P-148

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design and Synthesis of Ruthenium Aqua Complexes Featuring Oxidation Potential Inversion

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Series Ru-aqua complexes of $[\text{Ru}(\text{DAMP})(\text{BIAN})(\text{H}_2\text{O})]^{2+}$, where DAMP=2,6-bis(dimethylaminomethyl)pyridine and BIAN=Bis(arylimino)acenaphthene, were designed and synthesized for the study of oxidation potential inversion behavior. For the selection of target molecules, we employed DFT calculation method (B3LYP/cc-pVDZ/LANL2DZ//B3LYP/cc-pVDZ/LANL2DZ). Free energy differences between $\text{Ru}^{\text{II}}\text{-Ru}^{\text{III}}$ and $\text{Ru}^{\text{III}}\text{-Ru}^{\text{IV}}$ in the sequential two-electron proton-coupled oxidation reactions, $\text{L}_5\text{Ru}^{\text{II}}\text{-OH}_2 \rightarrow \text{L}_5\text{Ru}^{\text{III}}\text{-OH} \rightarrow \text{L}_5\text{Ru}^{\text{IV}}\text{=O}$, of more than 50 mononuclear Ru-aqua complexes were evaluated. BIAN ligands with five different aryl groups (phenyl, 4-tbutylphenyl, 4-methoxyphenyl, 4-bromophenyl, 4-nitrophenyl) were used for the systematic evaluation of electronic effect. Electrochemical experiments were performed to measure proton-coupled oxidation potentials and those data were compared with values predicted by theoretical calculations. These experiments provided useful benchmark to judge potential inversion behavior of Ru-aqua complexes for the design of future water-oxidation catalysts.

Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: **INOR.P-149**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Characterization of Tin Precursors for Atomic Layer Deposition of Tin Oxide Thin Films

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In the past decade, oxide semiconductor materials have attracted great attention for various applications in thin film transistors (TFTs), gas sensors, lithium batteries, and solar cells. Especially, tin(II) monoxide (SnO) which is a p-type material, has attracted material because of wide optical band gap energy (2.7~3.0 eV), which highlights the possibility of completely transparent electronic devices. Moreover SnO based TFT recently showed the record field effect mobility of $\sim 6.75 \text{ cm}^2/\text{V}\cdot\text{s}$ and Hall mobility of $\sim 18.71 \text{ cm}^2/\text{V}\cdot\text{s}$. On the other hand, tin(IV) dioxide (SnO₂) is an n-type material, which has also wide band gap energy ($\sim 3.6 \text{ eV}$) with excellent optical, electrical, and chemical properties. SnO₂ is transparent under visible light and the resistivity of SnO₂ films can vary at wide range. Doped SnO₂ films can be applied as transparent conducting electrodes. Generally, chemical vapor deposition (CVD) or atomic layer deposition (ALD) are required for uniform and conformal thin film growth. Moreover, SnO or SnO₂ can be deposited selectively by the oxidation state control with Sn(II) precursors and oxygen source. In the cases of ALD, various Sn precursor/reactant combinations have been studied to grow SnO or SnO₂ films, and many cases resulted in n-type SnO₂ films. So we have synthesized novel tin(II) complexes as potential precursors for ALD. The resulted complexes were characterized by various analysis equipments such as nuclear magnetic resonance (NMR), elemental analyses (EA), thermogravimetric analysis (TGA), and single crystal X-ray diffraction.

Conference Date: October 18~20, 2017

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Code: **INOR.P-150**

Area: Inorganic Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Tunable physical properties of redox-active porous coordination network via post-synthetic modification

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Porous coordination Networks (PCNs), known as reticular chemistry, which are constructed by connecting inorganic and organic units by coordination bonds. This material has attracted considerable attention due to their various kinds of application, such as gas storage, purification, catalyst, and electronic devices. However, sometimes it is difficult to produce proper pore environment because of many factors in chemical reactions. Post-synthesis modification can be a strong strategy to produce designable structure for target application. Herein, we report post-synthetic approach of redox-active PCN, which changed small diagonal channels to large opening pore, making accessible sites for metal and ligand exchanges by adding a solvent. This strategy enabled tuning the physical properties of redox-active PCNs.

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Area: Inorganic Chemistry

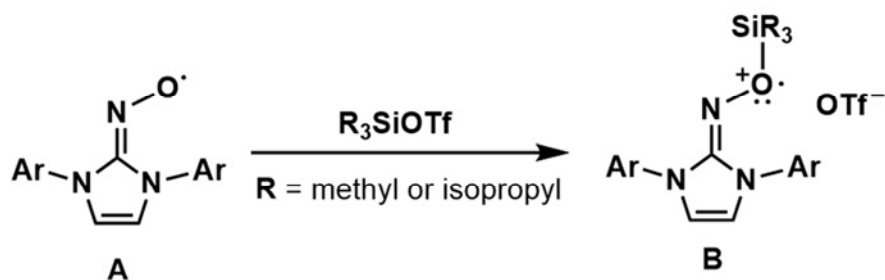
Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Silyl Oxime Ether Radical Cations Stabilized by N-heterocyclic Carbene

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N-heterocyclic carbenes (NHCs) are well known to stabilize main group radicals due to their π -conjugating effect [1]. Recently, our group reported the stable N-heterocyclic carbene nitric oxide (NHCNO) radicals A (Scheme 1), which can be also regarded as iminoxyl radicals stabilized by NHCs [2]. Interestingly, A reacts with series of silyl triflate to generate the corresponding radical cations B. The structures of the unprecedented silyl oxime ether radical cations were determined by X-ray crystallography, which revealed the delocalization of spin density through planar (imidazole ring)-N-O-Si group. Synthesis, characterization, and reactivity of the radical cations will be discussed. Reference [1] Song, H.; Kim, Y.; Park, J.; Kim, K.; Lee, E., *Synlett* 2016, 27, 477. [2] Park, J.; Song, H.; Kim, Y.; Eun, B.; Kim, Y.; Bae, D. Y.; Park, S.; Rhee, Y. M.; Kim, W. J.; Kim, K.; Lee, E., *J. Am. Chem. Soc.* 2015, 137, 4642.



Scheme 1. Synthesis of the silyl oxime ether radical cations stabilized by NHC.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-76**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Interpretations of behaviors of electronic/potential energy curves of highly excited Rydberg states of diatomic molecules in terms of generalized momenta in spheroidal (elliptical) coordinate systems by Gershtein et al's WKB method

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Highly accurate quantum chemistry calculations of highly excited Rydberg states are possible and have been routinely performed. They have been used to assign observed spectra of highly excited Rydberg states, usually with the united-atom designation. Such an assignment is sometimes ambiguous and undergoes reassignment several times, which derives from the lack in our knowledge on molecular Rydberg series. Calculation of quantum defect curves (QDCs) may resolve the ambiguity. The QDCs of several diatomic molecules have been calculated. Although they help us to identify Rydberg series, it becomes clear that currently there is no guiding principle for the assignment of Rydberg series, in particular, at the important chemical bonding region, for diatomic molecules with more than 4 electrons. The only guiding principle obtained from the study of one-electron diatomic molecules is the one applicable only in the region where core-splitting field is dominant. For this case, the semiclassical method by Hellmig long ago provides the satisfactory semi-quantitative theory. But his method has a fundamental singularity problem which was avoided with introduction of an arbitrary constant. The general theory for avoiding singularity problem was devised by Gershtein et al. I want use this method to replace Hellmig's method to handle the behaviors of Rydberg series.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-77**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study of the correlation diagram between united-atom and separated-atom states in HeH^+ by the quantum chemical multireference-configuration-interaction (MRCI) method and by the effective potential method in separable spheroidal coordinate systems proposed by Teller and Sahlin

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Surprisingly large probabilities of ionization in ion-atom collisions were explained with the promotion model using the correlation diagram between united-atom and separated-atom states by Fano and Lichten. Also correlation diagrams are used to assign molecular Rydberg spectra. Such diagrams were rather qualitatively constructed, in particular by Barat and Lichten, using the one in one-electron diatomic molecules obtained by Morse and Stueckelberg where diabatic and adiabatic potential curves are identical. But for molecular systems with more than one electron, they are not identical and it becomes clear that only correlation diagrams obtained by using the diatomic potential curves are meaningful. It is not a trivial problem and now it becomes widely known that the fundamental Smith's definition of diabatic states yields physically absurd results. The reason why diabatic and adiabatic curves are the same in one-electron systems is in the separability of Schrödinger equation in spheroidal coordinates. Teller and Sahlin proposed that effective potential method can be devised in Hartree manner in spheroidal coordinates and can thus be used for molecular systems with more than two electrons. Since the states obtained by this method is diabatic, it will be very interesting to compare the diabatic electronic curves obtained by this method and the one obtained by Smith's method with the inclusion of limited number of states to avoid the absurd physical results in the two-electron molecular system, HeH^+ .

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-78**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dynamics of mimic complex of [FeFe]-hydrogenase by using time-resolved wide angle x-ray scattering

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Water splitting to generate hydrogen becomes significant means of producing renewable energy and transporting energy. A number of efforts have investigated to synthesize and understand catalyst for the hydrogen evolution reaction and verify their reaction mechanism. One of the catalyst, hydrogenase, is the most active targets which is natural enzyme for hydrogen production. Hydrogenases can be classified as [NiFe], [FeFe] and [Fe] hydrogenase. One of those series has the active site containing the “butterfly” Fe_2S_2 group system which has been investigated in wide range. Roughly, our target complex has the bridging dithiolate species at binuclear iron metal centers, as well as six CO ligands. In this study, we demonstrate dynamics of $\text{Fe}_2(\mu\text{-S}_2\text{C}_3\text{H}_6)(\text{CO})_6$ using time-resolved wide angle x-ray scattering (TR-WAXS) measurements of 500 nm at the ID09B beamline of ESRF with 40 mM iron sample in acetonitrile. To support the experimental data and probe their kinetics, we have calculated optimized structure and MD simulation. To indicate multipath dynamics, we perform the global fitting. Our results show that the transient scattering intensities of $\text{Fe}_2(\mu\text{-S}_2\text{C}_3\text{H}_6)(\text{CO})_6$ complex is measurable although this complex does not contain any high-scattered atom. Our results have shown the reaction pathways occur upon excitation with UV or visible light which involves excitation to a short-lived ($\tau = 150$ ps) excited state with an elongated Fe–Fe bond. Another minor pathway involves a long-lived loss of a CO ligand within several μs .

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-79**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study of Manganese-Cobalt based Catalyst for Hydrogen Generation from Hydrazine monohydrate

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The Manganese-Cobalt composites (A-MnCo) are synthesized by a hydrothermal method under an aqueous basic condition and annealing process at 500 °C under hydrogen condition. The physicochemical properties of prepared powders are characterized by X-ray powder diffraction, high-resolution transmission electron microscope and X-ray photoelectron spectrometer. The XRD patterns of Manganese-Cobalt composites without annealing process (MnCo) represented the spinel structure ((Co,Mn)(Co,Mn)₂O₄). After being annealed, we confirmed that metallic cobalt and MnO are formed from mainly the spinel structures of MnCo. A-MnCo exhibits the TOF value of 14 h⁻¹ with 100 % selectivity for hydrogen generation from hydrazine monohydrate. However, MnCo does not act as catalyst for hydrazine decomposition. In addition, A-MnCo showed improved TOF value for the decomposition of hydrazine monohydrate compared with that of metallic Co (3 h⁻¹), and MnO (0 h⁻¹), respectively.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-80**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of copper-substituted Hydroxyapatite and application to dehydration of 1-octanol

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Hydroxyapatite (HAP, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) was synthesized using a hydrothermal method under basic aqueous conditions. Copper-incorporated HAP (CuHAP) was prepared by the ion-exchange reaction of HAP in aqueous Cu(II) solution. X-ray diffraction patterns and the morphologies of HAP and CuHAP were almost same. And inductively coupled plasma spectroscopy results indicated that the coppers are well dispersed on the surface of HAP. Therefore, we concluded that a monomeric form of coppers is randomly incorporated on the HAP. The catalytic activity of CuHAP was investigated for the dehydration of 1-octanol to dioctyl ether at 200 °C, 220 °C, 230 °C, respectively. The conversion of above reaction was 89% with selectivity to dioctyl ether of 53% at 230 °C.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-81**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Intramolecular charge transfer reaction dynamics investigated by femtosecond stimulated Raman spectroscopy

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4-Dicyanomethylene-2-methyl-6-p-dimethylaminostryryl-4H-pyran (DCM) is well known to form the intramolecular charge transfer (ICT) between the dimethylamino (donor) and the cyanomethylene (acceptor) in the excited states. Although DCM has been widely used in many fluorescence applications and many experimental and theoretical investigations have been performed, no experimental evidence on the structure of the ICT state such as “twisted” (in the dimethylamino or dimethylanilino group) and “planar” geometry has been revealed. In this work, the structural changes of DCM in the excited-state were directly observed by femtosecond stimulated Raman spectroscopy with both high temporal (

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-82**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Unveiling the Complexity of the Degradation Mechanism of Semiconducting Organic Polymers: Visible Light-Induced Oxidation of P3HT Films on ZnO/ITO under Atmospheric Conditions

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The oxidation of poly(3-hexylthiophene) (P3HT) films deposited on ZnO/ indium tin oxide (ITO) under blue light irradiation in either dry or humid atmosphere was studied using X-ray photoelectron spectroscopy in combination with UV-vis absorption spectroscopy. From results up to 12 h of reaction, ring-opening was hardly found and it is suggested that the water molecules chemisorbed competitively against O₂ (i.e., the major oxidizing agent), thereby decreasing the oxidation of P3HT. Beyond 12 h, thiophene ring opening took place at the topmost surface layer of P3HT, and the water vapor facilitated the ring opening of P3HT. Considering the oxidation in the entire polymer film, the humidity did not perform significant role on the oxidation behavior of P3HT. Here, the degree of oxidation of P3HT drastically increased when the reaction time exceeded 12 h. This suggests that the rate of oxidation of the entire P3HT film is determined by the slow diffusion of the activated oxygen species which was the major oxidizing agent into the deeper layers of the P3HT films. We also demonstrate that the photoinduced degradation of P3HT can be retarded by turning off light between irradiation, which may be due to the reversible desorption of activated oxygen species under dark conditions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-83**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The relation between the Hofmeister anions and water structure at protein surfaces

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Water has unique properties based on hydrogen bonding that is come from the specific atomic composition and molecular structure of water. These properties are crucial for the survival of life on the Earth. Thus, researched for water is highly important. Specially, we focused on these properties of water with protein and ions. To understand the relation between them, we carried out a molecular dynamics (MD) simulation. The result revealed that an effect of protein can affect ion distribution as well as water network only near the protein surface. And, the order of water network disruption followed the order of the Hofmeister anion series which is related with solubility of protein. Investigation for structural change of protein didn't show any significant change in our simulation. So, this result suggests that changes in the properties of the protein could originate from the disruption of the water H-bond network induced by ions with a higher affinity for the protein surface instead of direct protein residue-ion interactions. Additional investigation for orientational distribution of water molecules shows slight preference for interfacial water molecules, i.e. a straddle structure, within short ranges from the protein surface. Lastly, we found out that the cation effect on water network is also not negligible at the protein surface.

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Code: **PHYS.P-84**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Atomic dipole approximation for quantum plasmon simulation of nanoparticles

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Noble metal nanoparticles of which sizes are comparable to light wavelengths show characteristic colors due to the strong absorption/scattering of light in the visible region. Electromagnetic waves induce the collective oscillation of free electrons in the particles, which is referred to as localized surface plasmon resonances. Such an intriguing feature can be tuned by the size, shape, materials, and surrounding environments of nanoparticles for various applications in chemistry, physics, and biomedical fields. However, plasmonic nanoparticles in the quantum regime (1 ~ 10 nm) exhibit unusual optical properties that cannot be described by classical theories. Time-dependent density functional theory may serve as an effective and versatile tool for study on optical properties of such systems, but its application has been limited to very small clusters due to rapidly growing computational costs. For quantum plasmon simulations, we propose an atomistic dipole-interaction model which takes care of the interactions between induced dipoles with atomic polarizabilities purely obtained from TDDFT. Our new method shows very good agreement with TDDFT for plasmonic spectra of small silver clusters at much lower computational cost, though it is not appropriate for molecular-like excitations. In particular, it could remarkably reproduce the plasmonic band shift experimentally observed in sub-10 nm silver particles.

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Code: **PHYS.P-85**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Kinetic Study on Solvolyses of Thiophosphoryl Transfer Reactions

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The extended Grunwald-Winstein equation can be expressed as in equation (1) ; k and k_0 represent the specific rates of solvolysis of a substrate RX in a given solvent and in the standard solvent (80% ethanol), respectively; l is the sensitivity of the solvolysis towards changes in solvent nucleophilicity (NT); m is the sensitivity of the solvolysis towards changes in solvent ionizing power (YX, for a leaving group X); and c is a constant (residual) term. In this work, we investigated the solvolyses of phenyl 4-methylphenoxy thiophosphinyl chloride in pure solvents and mixed binary solvents to obtain an exact kinetic information in various solvents. $\log(k/k_0) = lNT + mYX + c \quad (1)$

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Code: **PHYS.P-86**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Protein Conformational Space Discretization by Using Thermodynamic Order Parameter

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Dimensionality reduction and clustering are commonly used for analyzing high-dimensional time-series data generated by atomistic biomolecular simulations. Their practical success depends critically on the choice of good order parameters or reaction coordinates. So far, geometric order parameters, such as the root mean square deviation from a reference structure, fraction of native amino acid contacts, and collective coordinates that best characterize rare conformational transitions, have been prevailing in the protein state space discretization. Here, we show that the solvent-averaged effective energy, which is unambiguously defined for a given protein conformation, serves as a good order parameter of protein folding. This is illustrated through the application to the folding-unfolding simulation trajectory of villin headpiece subdomain. The most distinctive feature of this thermodynamic order parameter is that it does not require any information on the native structure. We rationalize the suitability of the effective energy as an order parameter in terms of the funneledness of the underlying protein free energy landscape. We also demonstrate that an improved conformational space discretization is achieved by incorporating the effective energy. Because of its ab initio nature, the use of the effective energy will find wide applications in combination with unsupervised machine learning techniques.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-87**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Density Functional Study on Metal Ion Selectivity of Thiophene Derivative Compounds

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¹*Chemistry Education, Daegu University, Korea*

Recently, we have succeeded in synthesizing thiophene derivative compounds that show chemosenser behavior with several metal cations by synthesizing 2,2'-bithiophene-5-carbaldehyde and propane-1,3-diamine for synthesis of compounds.1 When the compound was mixed with various metal cations, such as Na(I), Cu(II), Ca(II), Zn(II), Co(III), Ba(II), Fe(II) and Fe(III), addition of Fe (III) showed strong fluorescence enhancement proportional to the concentration of Fe(III) as shown in Fig.1. In this study, we investigated the optimized structures of ligand compound and metal ion complexes through the quantum chemical calculation methods, such as B3LYP and LCgau-B97 which we recently developed.2 The quantum chemical analysis of the experimental results were carried out by calculating the uv-visible spectra and the applicability of the quantum chemical method to this field was examined.

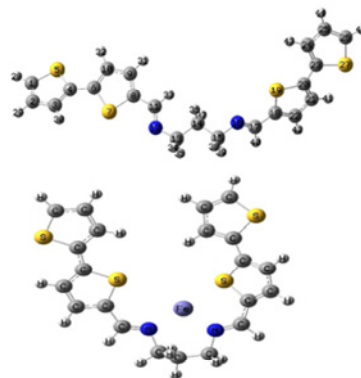
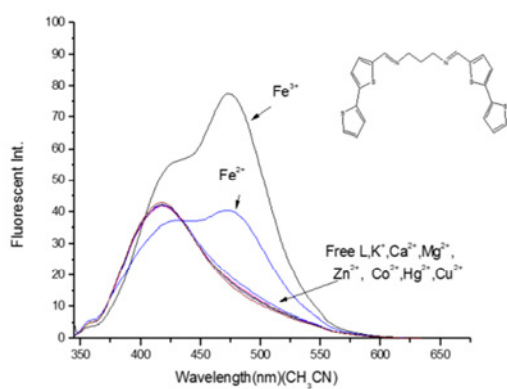


Fig.1 Fluorescent spectrum upon of various metal ion. - Fig.2 The structure of ligand and Fe(III) ligand

Complex compounds optimized using LCgau-B97.



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Code: **PHYS.P-88**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Quantum Chemical Investigations of Intermolecular Binding Energy between Carbon Nano-tube and Aromatic Molecules

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In this research, we have studied, by performing quantum chemical calculations, to find inter-molecular bonding strength between carbon nanotubes (CNT) and such molecules as aniline, benzophenone, and diphenylamine and favorable binding site on the CNT surfaces. Quantum chemical calculations were performed using B3LYP-D3/6-31G(d,p), which has shown high performances on intermolecular weak interaction calculations. We made the model of CNT structure (diameter: 1.97 nm) by cutting off to be an appropriate length and made each of the aromatic molecules adsorbed to the inside and outside of the CNT structure, performed the geometry optimization calculations and obtained the predicted binding energies. As the lengths of the CNT structure became longer, their binding energies increased slightly, but we found that their binding energies were converged at some predictable limit. The results of all the calculations were compared with the experimental data and it was confirmed that the quantum chemical calculations can explain the chemical phenomena observed in the experiment reasonably.

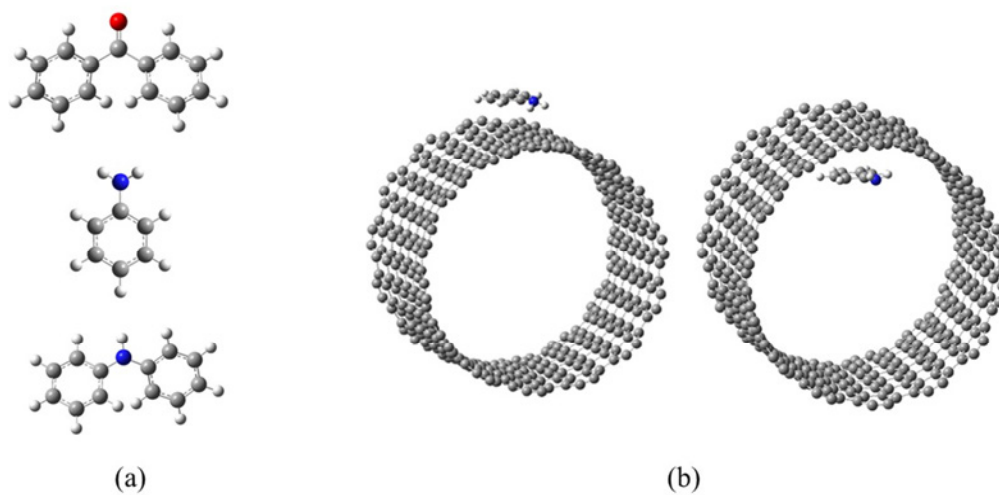


Figure 1. (a) aromatic molecules (b) aniline-adsorbed CNT structures optimized using B3LYP-D3/6-31G(d,p)



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Code: **PHYS.P-89**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Surface of Acidic and Basic Water

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Controversies on the acid-base properties of water surface were theoretically addressed with the help of large scale quantum mechanical molecular dynamics simulations (QMMD) on the water surface model systems with excess hydroniums or hydroxides. It was revealed that thermodynamic surface structures of these ions strongly depend on their surface location and dipole orientation. Hydronium is not only thermodynamically stable at the water surface, but it can also kinetically penetrate into the bulk via a fast proton transfer (PT) channel. On the other hand, the surface hydroxide is not as stable as hydronium. In addition, it can only take a slow molecular rotation as their major penetration mechanisms. Fast hydronium diffusion by PT establishes a wider kinetic depth distribution, while slow hydroxide is shallowly trapped below the outermost molecular layer (3~4 Å). On the basis of these, the enhanced acidity of water surface can be attributed in large part to the kinetic depth profile of the ion density in addition to static thermodynamic origin. Furthermore, the different depth profiles of the two ions may differently affect the surface-sensitive spectroscopic observations.

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Code: **PHYS.P-90**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Optical Properties for Bilirubin-Inducible Fluorescent Protein (holoUnaG)

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Bilirubin-inducible fluorescence protein (holoUnaG) was recently discovered and identified from eel muscle by the Miyawaki group. Fluorescence proteins like GFP have been used in a variety of biomedical researches. HoloUnaG of which size is smaller GFP is likely to be of use in studying biomedical and super-resolution researches. However, the optical and spectroscopic properties of holoUnaG have not been studied yet. For instance, even its fluorescence lifetime has not been clearly measured yet. Recently, we have carried out fluorescence lifetime measurement of holoUnaG in vitro and found that there are two fluorescence decay components, 2.2~2.3 ns and 0.8~0.9 ns. The relative amplitudes of these two components are about 80 and 20 %, respectively. It is believed that the slow component with 2.2~2.3 ns decay constant corresponds to the excited state lifetime of holoUnaG, whereas the fast component with 0.8~0.9 ns decay constant is from photo-damaged bilirubin or photo-isomerized bilirubin. We have also investigated the origin of significantly enhanced fluorescence intensity of holoUnaG as compared to those of either bovine serum albumin (BSA)-bilirubin complex or bilirubin molecule itself. Using electronic circular dichroism spectroscopy and quantum chemistry calculation methods, we were able to elucidate the mechanisms of fluorescence enhancement and extended lifetime of holoUnaG.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-91**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Determination of relative population of isomers of s-trans and s-cis crotonaldehyde on the neutral ground state by VUV-MATI spectroscopy and Franck-Condon factors

Sung Man Park, Hong Lae Kim^{*}, Chan Ho Kwon^{*}

Department of Chemistry, Kangwon National University, Korea

We measured vibrational spectra of trans- and cis-crotonaldehyde on the cationic ground state utilizing one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. The adiabatic ionization energy of the trans-s-trans isomer was determined to be 9.7501 ± 0.0004 eV, in excellent agreement with previously reported value, 9.75 eV. To interpret the observed VUV-MATI spectra, we performed the Franck-Condon simulation at the M062x/aug-cc-pVDZ level. As a result, we observed four different stereoisomers, trans-s-trans, trans-s-cis, cis-s-trans, and cis-s-cis in crotonaldehyde. From the VUV-MATI spectra and the Franck-Condon simulations, we were able to identify four different origin bands of each stereoisomer. In addition, we could determine relative population of the four isomers on the neutral ground state from the VUV-MATI spectra and the FC-factors. The measured population was very similar to the NMR data.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-92**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Structure and adsorption behavior depending on various pH conditions of 4',4''-(diazene-1,2-diyl)bis([1,1'-biphenyl]-4-carbonitrile) on silver surfaces

So Young Eom, Hong Lae Kim^{*}, Chan Ho Kwon^{*}

Department of Chemistry, Kangwon National University, Korea

Adsorption behavior of 4',4''-(diazene-1,2-diyl)bis([1,1'-biphenyl]-4-carbonitrile) (DDBBC) on silver surfaces was investigated depending on pH conditions to understand the surface-induced photoconversion between the amino group and the azo compound. The surface-enhanced Raman scattering (SERS) spectra of DDBBC on Ag surfaces were measured in various pH conditions as well as the ordinary Raman spectra of neat sample in solid state for comparison. Spectral assignments were provided with an aid of density functional theory calculations. In the SERS spectra, the up-shifted and the broadening of the CN stretching vibrational peak indicate that the adsorption takes place via the CN bond on the metal surface. However, the appearance of the C-H stretching bands and the disappearance of the N=N stretching (azo) bands in the acidic condition suggest that DDBBC should be converted to 4,4'-aminocyanobiphenyl adsorbed on the Ag surface with vertical orientation. In the present work, it is worth noting that the molecular structure and orientation against the Ag surface could be reversibly controlled by pH in solution.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-93**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

One-photon mass-analyzed threshold ionization spectroscopy of hydrazoic acid

Do Won Kang, Hong Lae Kim^{*}, Chan Ho Kwon^{*}

Department of Chemistry, Kangwon National University, Korea

We recorded for the first time the high- and low-resolution vibrational spectra of the cationic hydrazoic acid (HN_3^+) in the internal energy range of 0-1500 cm^{-1} by one-photon vacuum ultraviolet-mass analyzed threshold ionization (VUV-MATI) spectroscopy. The coherent VUV light was generated by non-resonant four-wave sum frequency mixing (FWSM) in a Xe and Ar mixture. The first ionization energy of HN_3 was determined to be $86591 \pm 5 \text{ cm}^{-1}$ ($10.7359 \pm 0.0005 \text{ eV}$) from the 0-0 band position in the MATI spectra, which is in good agreement with the literature values. We performed quantum chemical calculations to obtain vibrational frequencies and Franck-Condon factors at various levels and methods. In addition, we carried out the Franck-Condon fitting which utilized the cationic molecular geometry as fitting parameters for the simulated spectra to fit best to the experimental spectra. Almost all the peaks observed in the MATI spectra of HN_3 could properly be assigned based upon the calculated results. However, the observed split bands for each of the vibrational peaks in the high-resolution spectra seem to show rotational contours.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-94**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

SERS and DFT studies of 4-Aminobenzoic acid on silver surfaces in the presence of chloride anions

Do Geun Yoon, So Young Eom¹, Hong Lae Kim^{1,*}, Chan Ho Kwon^{1,*}

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We studied photo-induced dimerization of 4-aminobenzoic acid (4ABA) on silver surfaces in the presence of chloride anions. The dimerization took place by irradiation of the laser light and the reaction was completed within a few seconds. It is well-known that the chloride anion is a competitive adsorbate on the silver surface and can change the orientation of the probe molecules but we have not been able to confirm the orientation of the probe molecules. However, we confirmed that the dimerization did not occur in the experiment in which the chlorine ions were added. We compared these spectra with DFT calculations. The calculated spectra were in better agreement with the 4ABA spectra of the sol state than the spectra presented in the previous work.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-95**

Area: Physical Chemistry

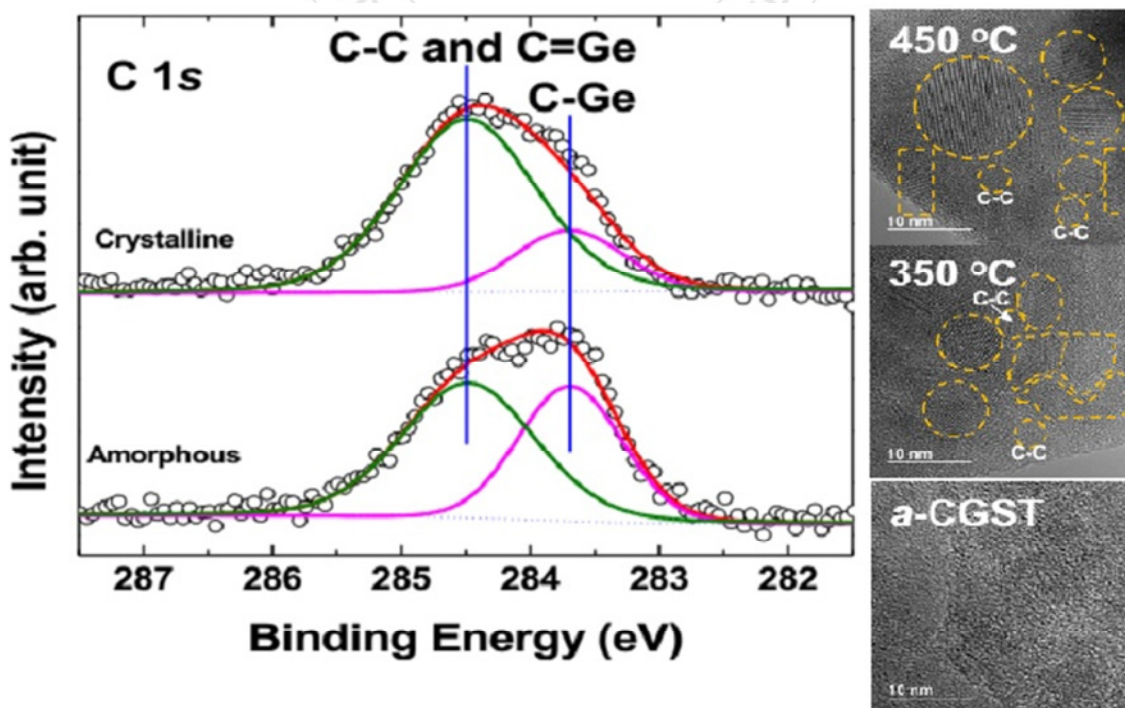
Type: Poster Presentation, Time: FRI 13:00~14:30

Formation of deep chemical bonding between C and Ge in C (C: 1.5 wt.%) doped $\text{Ge}_2\text{Sb}_2\text{Te}_5$ after phase-change

Young Mi Lee

Beamline Department, Pohang Accelerator Laboratory (PAL), Korea

C doped (1.5 wt.%) GST (CGST) thin film was formed on Si substrate by using sputter method with 100 nm-thick and confirmed resistance, atomic structure, and chemical state of CGST. From exploring chemical states of amorphous and crystalline CGST, we found the C-C bonding with cluster structure/Ge-C bonding and the deep double bonding (Ge=C) in amorphous and crystalline phases, respectively. The reverse-relationship between Ge-C and Ge=C bonds in amorphous and crystalline phases is observed in the analysis of chemical states.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-96**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids

YoonJae Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Liquids consist of regions of different mobility near the glass transition, which is called the dynamic heterogeneity. Particles in glass-forming liquids may form domains of locally favorable structures (LFS) upon supercooling. Whether and how the LFS domains would relate to the slow relaxation and dynamic heterogeneity of the glass-forming liquids have been issues of interest. According to the Stokes-Einstein (SE) relation and the Debye-Stokes-Einstein (DSE) relation, the ratio of the translational (D_T) and rotational (D_R) diffusion coefficients should be a constant over a range of temperatures. In supercooled liquids and glasses, however, D_T and D_R decouple due to dynamic heterogeneity, and D_T/D_R may not be constant any more. In this study, we employ tracers whose structures resemble the LFS domains in Wahnström and Kob-Andersen (KA) glass-forming liquids, and investigate the translation-rotation decoupling of the tracers. In Wahnström liquids, icosahedron LFS domains are the most long-lived ones and the mobility of neighbor particles is suppressed. We find from our simulations that the icosahedron tracers experience drastic translation-rotation decoupling upon cooling. In KA liquids, bicapped square antiprism LFS domains are the most long-lived ones, which are not correlated significantly with the local mobility. D_T and D_R of bicapped square antiprism tracers do not decouple significantly. The difference in the decoupling behavior between different types of tracers indicates that there should be the structural motif during in glasses.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-97**

Area: Physical Chemistry

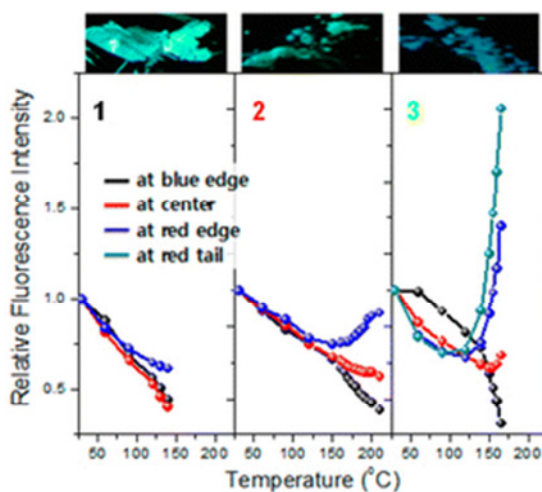
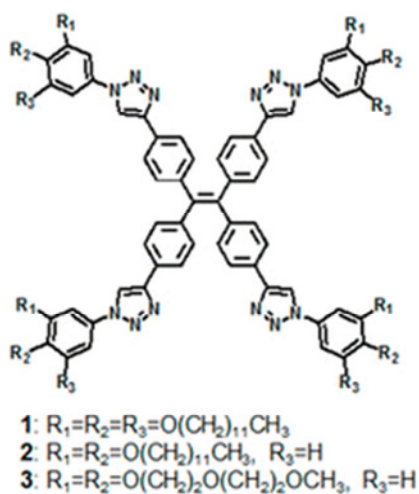
Type: Poster Presentation, Time: FRI 13:00~14:30

Advantages of Mobile Liquid-Crystal Phase of AIE Luminogens for Effective Solid-State Emission

Hoa Thi Bui, Sung Cho^{*}

Department of Chemistry, Chonnam National University, Korea

We investigate aggregation-induced emission (AIE) characters of bulk tetraphenylethene (TPE) derivatives with nonpolar and polar exterior chains. The bulk TPE derivatives with nonpolar dodecyl and polar di(ethylene oxide) chains are in liquid crystal (LC) and crystalline phases, respectively, at room temperature. The mobile LC character of the TPE derivatives in bulk is crucial for high AIE efficiency because the mobile LC character is effective in minimizing the number of undesirable nonemissive local sites in aggregates and inducing a homogeneous zigzag-stacked columnar structure with j-type coupled transition dipoles of the TPE derivatives. The mobile LC characteristics of AIE luminogens can be advantageous for highly efficient solid-state emission.



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Code: **PHYS.P-98**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Small Molecule Solvatochromism with Alkyne-Tagged Vibrational Probe

You Na Kim, MINHAENG CHO*

Department of Chemistry, Korea University, Korea

It is important to understand the solvatochromism of Raman imaging, because it can be used to observe small molecules by detecting molecular vibrations and has better spatial resolution than IR imaging. To observe the small molecules, recent Raman imaging experiments attach labels to target molecules, which is called Raman tag imaging. This method can be used to observe the Raman spectra of molecules in the silent region. The silent region is 1800 to 2800 cm^{-1} and certain functional groups show the Raman band in this region. Among the various functional groups, alkyne vibrations provide clear and strong Raman spectra in silent region. In Raman imaging, the alkyne probe can be used to explore the surrounding environment of the molecule through frequency shifts according to solvatochromism. We will show $\text{C}\equiv\text{C}$ stretch frequency shifts distributions obtained by combining the SoleFP/HF/6-311++G** method with molecular dynamics simulation and compare with the $\text{C}\equiv\text{C}$ stretch frequency shift components that were computed for various propargyl alcohol-(H_2O) $_n$ clusters using ab initio(HF/6-311++G**) method.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-99**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dynamics of Ligand Rebinding to Cytochrome using Time-resolved Infrared Spectroscopy

JuHyang Shin, Manho Lim^{*}, CheongHa Lim¹

Department of Chemistry, Pusan National University, Korea

¹*Pusan National University, Korea*

Femtosecond and nanosecond vibrational spectroscopy was used to probe the rebinding dynamics of CO to cytochrome (Cgb) after photodissociation of the corresponding CO-bound protein in D₂O buffer (pD = 7.4) at 273 K. When excited with a 532-nm photon, carbon monoxide dissociated immediately from cytochrome (< 0.2 ps), ground state bleaching of CO bound to the cytochrome has three conformations (A0, A1 and A3). Each conformation shows characteristic ¹³C–O stretching frequencies. The vibrational spectrum of CO in CgbCO described three gaussians at 1924 cm⁻¹ (A0), 1899 cm⁻¹ (A1) and 1884 cm⁻¹ (A3) with a full width at half-maximum (FWHM) of 15 cm⁻¹, 18 cm⁻¹ and 12 cm⁻¹. Ligand binding to Cgb is a multiphasic process with fast geminate rebinding taking place on the nanosecond timescales and slower biomolecular rebinding occurring on microsecond timescales.

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Code: **PHYS.P-100**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Conformation-dependent Photodissociation Dynamics of C₂F₄I₂ in Solution

Seongchul Park, Manho Lim^{*}, Youngshang Pak

Department of Chemistry, Pusan National University, Korea

Photodissociation dynamics of CF₂ICF₂I in solution was investigated by probing the C–F stretching mode using femtosecond mid-IR pulse after excitation with a femtosecond 267-nm pulse. Dissociation of the first I atom was faster than 0.3 ps after the UV absorption. All of the resulting haloethyl radicals undergo the secondary dissociation with two time constants forming CF₂CF₂; the radical from the anti-CF₂ICF₂I, the major conformer with c.a. 80% population in CCl₄ or in CH₃CN solution dissociates with time constant of 165 ps or 42 ps, respectively. The radical from gauche-CF₂ICF₂I in CCl₄ or in CH₃CN solution dissociates with the time constant of 4.2 ns or 3.5 ns, respectively. The dissociation time is slower than 25 ps, time constant for the presumably major conformer in the gas phase. However, the estimated quantum yield (QY) for the secondary dissociation in solution was found to be 1, which is higher than the reported value much less than 1 in the gas phase. Previously the secondary dissociation QY in solution was reported to be 0.3 ~ 0.95. A photodissociation mechanism that explains the conformer-dependent dissociation rate of CF₂ICF₂I as well as its solvent-dependent dissociation rate is presented based on a potential energy surface of CF₂ICF₂ radical calculated with CASSCF.

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Code: **PHYS.P-101**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Ultra-small Pd Nanoparticles Deposited on CdS Nanorods by Pulsed Laser Ablation in Liquid: Role of Metal Nanocrystal Size in the Photocatalytic Hydrogen Production

Hanbit Park, Amaranatha reddy, TaeKyu Kim*

Department of Chemistry, Pusan National University, Korea

It is essential to suppress the recombination rate of photogenerated carriers for the improvement of semiconductor-catalyzed solar-driven hydrogen production. To that end, photocatalysts comprising active sunlight-harvesting photoabsorbers and stable metal co-catalysts have attracted significant attention. However, the size, clean surface, and highly dispersed nature of the metal co-catalysts are crucial factors affecting the catalyst performance and reaction rate. Nevertheless, most of the available metal nanocrystals have been synthesized using complex procedures and harmful organic templates and stabilizers, affording high-purity compounds with difficulty and high cost. To overcome this difficulty, in this study, the pulsed laser ablation in liquid approach was utilized to generate Pd and bimetallic PdPt nanoparticles with an average size and distribution by adjusting the laser wavelength and fluence. A high hydrogen evolution rate of $130.33 \text{ mmol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ was obtained using the optimized CdS-PdPt catalyst under simulated sunlight irradiation. This value is 51.31 times greater than that observed for bare CdS nanostructures. Furthermore, the amount of evolved hydrogen was significantly better than that obtained using several noble-metal co-catalysts deposited on CdS. This proposed strategy is thought to open new strategy for designing advanced photocatalytic materials for efficient solar-driven hydrogen production.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-102**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Catalytic activity of Fe₂O₃ nanoparticles deposited on mesoporous Al₂O₃ bead toward toluene combustion

CHANHEUM PARK, IL HEE KIM, Sangwook Han, Ho Jong Kim, BYEONG JUN CHA, JAEHWN JEONG, TaeGyun Woo, Hyun Ook Seo¹, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

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

By temperature-regulated chemical vapor deposition (TR-CVD), Fe₂O₃/Al₂O₃ and NiO/Al₂O₃ catalysts were made using ferrocene, nickelocene vapor as metal precursor and air as oxidizing agent, respectively. While NiO/Al₂O₃ showed narrow distribution of NiO nanoparticles with only shell part which of depth were ~50 nm, Fe₂O₃ nanoparticles could be distributed even at the core part of Al₂O₃ bead. After post-annealing of these catalysts under air at 450-750 °C, these catalysts were used for total oxidation of toluene in the reaction temperature range of 150-350 °C. Fe₂O₃/Al₂O₃ showed significantly higher catalytic activity than NiO-based catalysts, which can be attributed to the wide distribution of Fe₂O₃ nanoparticles, i.e., very small catalytically active nanoparticles are distributed in the entire structure of the mesoporous supporting material. 100% conversion of toluene into CO₂ with a long-term stability of the catalytic activity was realized at 350 °C using Fe₂O₃/Al₂O₃ under both dry and humid conditions with a toluene concentration of 10,000 ppm in the feed gas. It is worth noting that the unique structure of the Fe₂O₃/Al₂O₃ is stable after air-post-annealing at 750 °C. Our Fe₂O₃/Al₂O₃ catalysts are active for toluene oxidation, and stable upon annealing at high temperature, showing that one can use our catalysts as a component of catalytic converter of harmful volatile organic compounds.

120th KCS General Meeting & Exhibition

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Code: **PHYS.P-103**

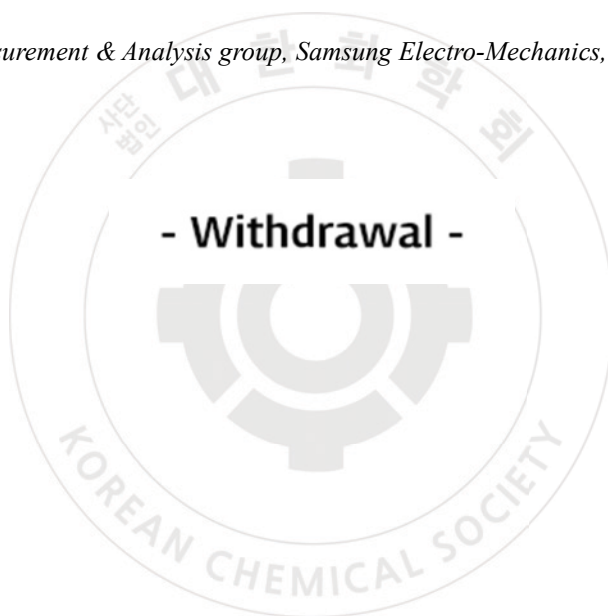
Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

[Withdrawal] Crystalline structure analysis of carbon materials with micro-Raman spectroscopy

Junghwa Lee

Measurement & Analysis group, Samsung Electro-Mechanics, Korea



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-104**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

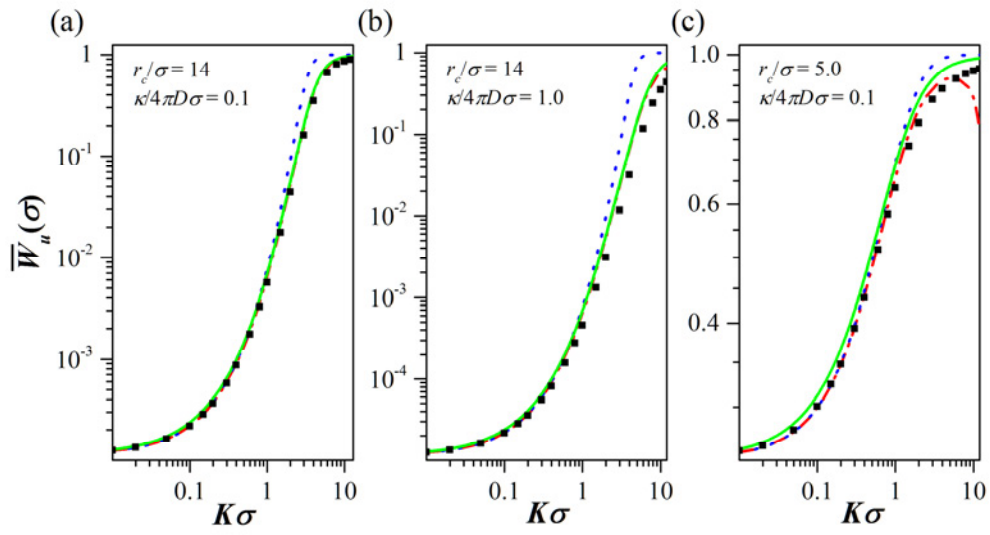
Effects of External Electric Field and Anisotropic Long-Range Reactivity on Charge Separation Probability

Kyusup Lee, seonghoon lee, Cheol Ho Choi¹, Sangyoub Lee*

Department of Chemistry, Seoul National University, Korea

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

We consider the effects of external electric field and anisotropic long-range reactivity on the recombination dynamics of a geminate charge pair. A closed-form analytic expression for the ultimate separation probability of the pair is presented. In previous theories, analytic expressions for the separation probability were obtained only for the case where the recombination reaction can be assumed to occur at a contact separation. For this case, Noolandi and Hong obtained an exact solution, but their expression for the separation probability was too complicated to evaluate. Hence an approximate analytic expression proposed by Braun has been widely used. However, Braun's expression overestimates the separation probability when the electric field is large. In this work, we present an approximate analytic expression that is simple and accurate enough for all parameter values. In addition, the expression is also applicable when the interaction between the geminate charge pair is described by screened Coulombic potential, and the recombination reaction has an anisotropic and long-range reactivity. We also provide the expression for the separation probability when the initial separation between the geminate charge pair is larger than the contact distance.



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Code: **PHYS.P-105**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Systematic Ligand Modification of TM Complexes for Improved Redox Potentials

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Department of Chemistry, Sungkyunkwan University, Korea

¹*Department of Chemical Engineering, Sungkyunkwan University, Korea*

An electrolyte with redox potential as high as possible is one of the important properties of an efficient redox flow battery (RFB) material. Many systems have been considered for this application including organometallic complexes. Such systems have the benefit of a metal center that can handle several oxidation states and an organic ligand which can be modified to attain desired increase in reduction potential (E^0). In this study, a series of first row transition metal ($M = \text{Cr, Mn, Fe, Co, Ni}$) complexes with known E^0 were systematically modified via its ligand by adding electron donating (EDG) and withdrawing (EWG) groups. Using DFT calculations we found that EDG such as $-\text{NH}_2$ will cause a negative shift in E^0 while EWG have the opposite effect. The overall trend of the calculated E^0 s according to ligand modifications were predicted to have the order as $-\text{NH}_2 < \text{Pristine} < -\text{F} \approx -\text{CN} < -\text{NO}_2$. In addition, optimized geometries, LUMO, vertical electron attachment and energy components constituting E^0 were discussed in detail to assist the further understanding for E^0 s. Consequently, we suggested that 16 complexes can play a role as a catholyte in aqueous redox flow battery. Especially, it is expected that $[\text{MnL}_\text{F}]$, $[\text{MnL}_\text{CN}]$ and $[\text{NiL}_\text{NH}_2]$ can be used as promising catholyte candidates possibly possessing high E^0 s which almost reach to the reduction potential limitation 1.25 V in aqueous redox flow battery. Our systematic approach to tune E^0 can be applied to the design other complexes via rational ligand modification.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-106**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Noninvasive, Layer-selective Analysis of OLED Degradation

**JUNGBAE SON, JOO YOUN KANG, Sohyeon Bae, Key Young Yang¹, Jongseok Han²,
Changhee Lee², Seong Keun Kim^{*}**

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¹*Department of Electrical and Computer Engineering, Seoul National University, Korea*

²*Seoul National University, Korea*

Despite the importance of understanding the ultimate cause of the degradation of organic light-emitting diodes (OLEDs) and identifying the specific layer responsible for such degradation, much is not known to date. To examine individual layers of an OLED device for degradation and identify the culprit for OLED degradation, we devised a noninvasive, layer-selective analysis method. We designed an OLED panel whose 3 layers (for electron transport, emission, and hole transport) have distinct emission wavelengths and thus can be discriminated from one another. We measured the photoluminescence intensity and lifetime of each layer as the OLED panel was subject to electro-degradation. We were able to spectrally separate layers and found different degradation features of each layer. This method is highly suited for noninvasively analyzing the mechanism of electro-degradation and the change occurring in each layer as a result.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-107**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Raman Spectroscopic Approach to Photo-Degradation Process of PTB7-Th Polymer

sangjun Kim, Kyusang Ahn, kyungwon Kwak^{*}, MINHAENG CHO^{*}

Department of Chemistry, Korea University, Korea

Organic photovoltaic(OPV) is one of the most promising chemical components due to its potential to becoming next generation solar cell such as low cost, flexibility etc. Because of its potential, OPV has been studied to improve the power conversion efficiency. However, there is the Achilles heel of OPV, photodegradation. Even in the ambient condition, the stability of OPV is much lower than silicon based solar cell. In this research, we use our home-built Raman spectroscopy to observe the photodegradation process of PTB7-Th in molecular level. As a result, we found that during initial degradation process, two distinct phase are observed (Phase I, Phase II). In Phase I, oxygen is the crucial role in degradation. By using DFT calculation, we could find the place where the degradation occurs. In Phase II, water determines the rate of degradation. We hope this research would be the clue to find the valuable information during photodegradation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-108**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Coil-globule Transition Pathway Determines the Structure of a Polymer Globule as a Model for Chromatin Organization

Seulki Kwon, Bong June Sung^{*}

Department of Chemistry, Sogang University, Korea

Chromatin undergoes a condensation-decondensation process repeatedly during its cell lifetime. The spatial organization of chromatin in nucleus resembles the fractal globule, whose structure significantly differs from an equilibrium polymer globule. There have been efforts to develop a polymer globule model to describe non-equilibrium and fractal structure of densely-packed chromatin in nucleus. However, the transition pathway of a polymer toward a globular state has been often ignored. Because biological systems are intrinsically non-equilibrium and largely fluctuating, it matters what transition pathway the chromatin would take before reaching the densely-packaged globule. Moreover, the transition pathway might affect the final globular structure substantially. In this study, by using a simple polymer model and Langevin dynamics simulations, we investigate the conformational transition of a single polymer from swollen coil to compact globule in order to elucidate the effect of transition pathway on the final globular structure. We consider three representative thermodynamic variables that induce coil-globule transition: T (temperature), V (volume of the system), and N (the number of particles in the system). The structure of polymer globule could be characterized by the probability ($P(s)$) of contact between two loci separated by a distance s . We show that a fast collapse induces a non-equilibrium fractal-like structure, whose relaxation toward an equilibrium globule is extremely slow. Moreover, with high confinement, it never relaxes into equilibrium state, thus the structure of the globule becomes dependent on the transition pathway.

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Code: **PHYS.P-109**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Reduction of 4-Nitrophenol to 4-Aminophenol : Boosting Catalytic Efficiency by Coupling with Copper via Liquid Phase Pulsed Laser Ablation

YUJIN KIM, Hanbit Park, Rory Ma, Amaranatha reddy, TaeKyu Kim *

Department of Chemistry, Pusan National University, Korea

Ultra-dispersed bimetallic nanomaterials have attracted much attention in the reduction of highly toxic aromatic nitro compounds to aromatic amines owing to their high stability, superior activity, reusability, and unique optical and electronic properties, as compared to monometallic nanocrystals. However, the lack of facile strategy of producing highly pure ultra-dispersed bimetallic nanocatalysts limits their practical industrial applications. Considering the above obstacles, we present a simple and effective strategy for the formation of bimetallic (PdCu) nanocrystals by liquid phase pulsed laser ablation using a bulk Pd metal plate submerged in CuCl_2 solution with different concentrations. The microstructural and optical properties of the synthesized nanocrystals indicate that the obtained bimetallic nanostructures are highly pure and monodispersed. Moreover, bimetallic PdCu nanostructures show a higher catalytic activity than monometallic Pd nanocrystals for the hydrogenation of 4-nitrophenol to 4-aminophenol at room temperature, also exhibiting high stability for up to 4 recycles. Finally, we believe that the presented strategy and utilization of bimetallic nanocrystals for catalytic applications enable the development of novel bimetallic nanostructures produced by liquid phase pulsed laser ablation and their catalytic application for environmental remediation.

Conference Date: October 18~20, 2017

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Code: **PHYS.P-110**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Vibrational predissociation of aniline-methanol-water cluster cation

HyunWook Choi, Jae Kyu Song, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

Molecular structure and photodissociation of aniline-methanol-water cluster cations (AnMeW_2^+) have been investigated by linear tandem time-of-flight mass spectrometer. Mass-selected AnMeW_2^+ cluster was irradiated by infrared laser ($2800 - 4000 \text{ cm}^{-1}$). Intense peaks were observed around 2990, 3200, 3430, and 3680 cm^{-1} in the infrared action spectrum, which were assigned NH_2 symmetric, asymmetric stretching, bounded water symmetric stretching, and unbounded water symmetric stretching mode, respectively. Optimized structures and theoretical infrared spectra of AnMeW_2^+ were also calculated by the Gaussian 09 program at the M06-2X/cc-pVTZ theory level.

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Code: **PHYS.P-111**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Effect of Small Group Discussion Class Based on Social Constructivism on Perception of Evaporation and Boiling by Pre-service Chemistry Teachers

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summaryThe purpose of this study was to examine the perception of pre - service teachers about the concepts of evaporation and boiling and to analyze the narrative contents of elementary, middle and high school textbooks affecting their perceptions and then to experience small group discussion class based on social constructivism, Concept change. And I analyzed the contents of pre - service teachers who experienced the concept change perceived by the social constructivist class. First, it was necessary to recognize difference of preconditions in the concept of science, second, importance of consensus among teachers, and third, recognition of teacher 's conflict as knowledge transferor. This study suggests that experiencing the consensus process through social constructivism when teaching the concept of science will have a very important educational effect in the pre - service teacher education. Key words: evaporation, boiling, social constructivist, consensus, open, closed, equilibrium, unbalancedIntroductionThe need for researchIn social constructivism, we see that scientific knowledge explaining natural phenomena is constituted through social consensus (Bentley et al, 2000), and knowledge is formed within a specific community. The main factors in determining the validity of knowledge in the composition of scientific knowledge are socio - political processes and knowledge is seen as socially agreed knowledge. Therefore, teachers should understand and teach science concepts in the context of social consensus and context, rather than conveying the knowledge described in textbooks. It is not about getting students to memorize or memorize the scientific knowledge that is described in the textbook or the teacher's message, but to share and discuss their own knowledge and understand and construct knowledge again. Therefore, in order to understand and acquire concepts correctly, constructivism that constructs concepts and internalizes them must be reflected in education. Research methodTheoretical backgroundIn this respect, constructivists pursue new knowledge that is formed in a

context of variable reality, rather than a search for fixed invariant truths (eg, Park, 2010). In the previous research, the definition of science knowledge is conceptual and socially constructed rather than value-centered, and the theories of science can also be interpreted as contextual rather than absolute (2007). Intervention and negotiation with an authority is indispensable if the learners' acceptance is scientifically changed. In this regard, the professor is learning soon (Jo, Yeon-ju, 1998, p392-18-19). It is necessary to suggest a step to recognize scientific terminology. It is analyzed that the concepts presented as the conditions of the state change are not presented as the particle concept that is the microscopic concept level but can be misconceptions when presented at the macro level. It should be redefined to clearly define the terms, to present the relevance between concepts, and to describe them in an integrated way.

Research method
Selection of research topics → Study of previous studies → Preparation of questionnaires → Input of preliminary questionnaires → Pre-interview with preliminary teachers in questionnaires → Analysis of textbooks → Analysis of questionnaires and interview data → Conducting small group discussion class based on social constructivism → Putting in after questionnaires → Preparation after class Interview with teachers → Analysis of results → Conclusion

Research results and discussion
As a result of discussing for social consensus, we showed a reflective attitude toward the existing concept of science learning, which considers the expression of the reference boiling point in the picture of equilibrium, without considering the concrete conditions of the boiling phenomenon. In addition, small group discussions based on social constructivism are influenced by other pre-service teachers and cause the transition of thinking. Pre-service teachers need to reconstruct their knowledge in order to understand the knowledge accurately. In addition, There was a lot of discussion in the process of defining the term 'boiling' in order not to inject knowledge but to understand it not to form the same concept as oneself. Once an agreement has been reached between teachers on the definition of terms, it is likely that they will be able to teach students the equivalent concept. In the process of expressing the concept with Venn diagram, it showed that there is a difference in the way of expressing one's own thoughts. The perception of these inconsistent expressions was evident in the discussion process, and the role of this discussion process helped teachers to recognize the need for consensus in social constructivism. Therefore, in the future, it is necessary to show the difference of perception about the precondition in elementary, middle, and high school education when dealing with the concept of science in pre - service teacher education, , Which will be an important contribution to the acquisition of the educational knowledge needed to guide students to science concepts.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-112**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Exponential Law for Complete Basis Limit of CCSD(T) Theory for OH Vibrational Potential Energies of Water Molecules

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Quantum chemical electronic energy of a molecular system depends on the level of the employed basis functions. The exponential laws describing the convergences of the calculated Hartree-Fock (HF) and electronic correlation energies of water molecules have been determined by fitting the energies predicted by the CCSD(T) theory with various levels of correlation consistent basis functions. The law was applied to calculate the energies of a few simple water clusters by varying the OH bond distance of a molecule in order to understand how the two parts of the potential energy subject to the stretching motion of water molecules depend on the variation of local environments. It is found that the HF energy strongly depends on the environments of a local OH bond while the correlation energy is almost insensitive to the neighboring molecules. This suggests that the HF theory may have a great advantage in saving computation time for efficient calculations of vibrational frequencies widely distributed due to the inhomogeneity in the local environments of water molecules in the condensed phases.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-113**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Photophysical properties of dyes in reverse micelles studied by time-resolved electronic spectroscopy

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Proton transfer or charge transfer is known as one of important chemical processes in many chemical and biological systems. Photo-induced proton and charge transfer occurring on ultrafast time scales have been of great interest in time-resolved spectroscopy. HPTS (8-hydroxypyrene-1,3,6-trisulfonic acid) is one of well-known photoacids. Its pKa value decreases greatly ($7.7 \rightarrow 0.5$) when photo-excited and deprotonated HPTS shows distinct emission spectrum and kinetics compared to those of protonated HPTS. Another molecule is DNBP (4-Dimethylamino-4'-nitrobiphenyl) whose geometry in the ground state has a torsional angle of ~ 40 degree between two phenyl rings. Upon the photoexcitation, excited-state charge transfer occurs with the rotation of phenyl rings which are strongly dependent on the solvent polarity and viscosity. Emission spectra of DNBP show large Stokes shifts in polar solvent than nonpolar solvent. In this research, excited-state dynamics of HPTS and DNBP were investigated by time-correlated single photon counting (TCSPC) and femtosecond transient absorption spectroscopy. Fluorescence of HPTS and DNBP are strongly affected by solvent properties and local environments; dyes encapsulated in nano-pools of reverse micelles showed significant difference in emission spectra and kinetics compared to those in bulk phase. Emission spectra of HPTS in reverse micelles show a large change in the ratio of deprotonated species depending on the size of the nano-pools. Also emission spectra of DNBP in reverse micelles shift between the emission spectra of polar and nonpolar solvent. In addition, quantum yields of DNBP in the reverse micelles increase dramatically against the bulk phase.

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Code: **PHYS.P-114**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Surface Adsorption of Hydroxyanthraquinones on CTAB-modified Gold Nanosurfaces

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Adsorption of organic molecules onto metal nanosurfaces makes their Raman signal dramatically enhanced. It is called surface enhanced Raman spectroscopy (SERS), and spectral features of SER signal can provide detailed information on the surface adsorption geometry of a molecule on the metal surfaces. In this research, gold nanoparticles were used to obtain SER spectra of hydroxyanthraquinones (HAQs), and cetyl trimethylammonium bromide (CTAB) was used as a cationic co-adsorbate. When concentration of CTAB was optimized, sample color was turned abruptly, and SER signals of HAQs were dramatically enhanced. CTAB seems to make HAQs aggregated with gold nanoparticles, which is in line with an increase of absorption in longer wavelength region upon adding CTAB solution. Signal of alizarin SERS was gradually increased as pH of the sample increases, and this tendency supports that deprotonated alizarin can readily be adsorbed to gold nanoparticles whose surface is modified with CTAB. Two distinguishable SER spectra occurred upon changing pH imply that there are two or more aspects of adsorption geometry of alizarin on the gold surfaces modified with CTAB.

120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

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Code: **PHYS.P-115**

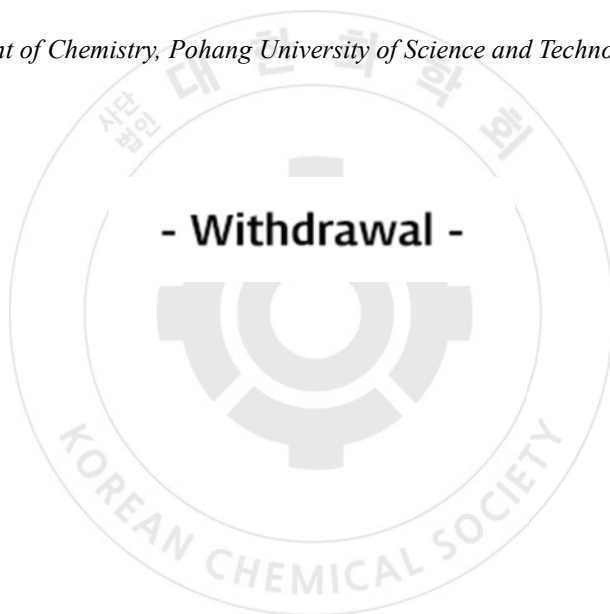
Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

[Withdrawal] Crystallographic Orientation-Dependent Raman Spectra of Layered CrPS₄

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Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-116**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fundamental Raman Study of Single and Few layer ^{13}C Graphene

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^{13}C graphene has different lattice vibration frequencies than its isotopologue ^{12}C graphene because of difference in their atomic masses. While the Raman scattering of single and multi-layer ^{12}C graphene has been extensively studied during the past decade, the same statement can hardly be made for ^{13}C graphene. In this work, we systematically investigated the Raman scattering of single and multi-layer ^{13}C graphene prepared by mechanical exfoliation of ^{13}C graphite. As the number of layers increased, G peak grew in intensity and the line shape of 2D peak converged to that of ^{13}C graphite. Based on the G peak intensity and line shape of 2D peak, the thickness could be reliably determined from single to 8 layers. To establish Raman metrology for lattice strain and charge density of ^{13}C graphene, extensive Raman mapping was performed and lead to a quantitative correlation between G and 2D frequencies. To determine the dispersion of 2D frequency as a function of excitation energy, bilayer ^{13}C graphene was probed at various excitation energies of 1.96, 2.41 and 2.71 eV. As excitation energy increased, the 2D peak up-shifted because excitation energy affects the vibration mode selected during the process of double resonance. This work will expand the utility of ^{13}C graphene in various research and applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-117**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Infrared spectroscopy of Electrolyte in Lithium-Ion Batteries

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Lithium ion battery(LIB) is indispensable material in daily life for the portable energy storage devices. For this reason, various studies of LIB have been steadily done specially to increase the efficiency and stability. To find out the maximum efficiency condition of battery, researchers measure the conductivity by exchanging component of electrodes and electrolytes. According to various measurements and researches, it is believed that molecular details are essential to understand the chemistry inside of the LIB. In other words, small changes in molecular structure seems to affect much to the performance of LIB. Moreover, these observations can't be explained by macroscopic physical properties like dielectric constant or viscosity. To study these phenomena, we observe microscopic interaction of electrolytes, how solvent molecules interact with lithium ion and how they transfer it, and how these results influence on the conductivity of battery therefore. For this study, we use infrared spectroscopy because infrared absorption is highly sensitive to the change of environment around Li⁺ ion. With salt concentration dependence, mixing ratio between main and co-solvent, and investigation low frequency mode, we can investigate the effect of salt exchange and solvent exchange. This will provide molecular information about the electrolytes for new advanced battery system.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-118**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Metal-enhanced Fluorescence Observed with Homogeneous Silver Colloidal Films

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The emission of dye molecules is largely enhanced by noble metal nanoparticles due to locally-enhanced electric fields and surface plasmon coupled emission (SPCE), which is in general called metal-enhanced fluorescence (MEF). MEF has been extensively applied to many disciplines including biological sensing and imaging, and organic optoelectronics but the details of the MEF are not yet clear. In this study, we fabricated homogeneous silver colloidal films (SCFs) composed of silver nanoparticles in a wide range of diameter (70-200 nm). The extinction spectra of homogeneous SCFs showed spectral shifts depending on the size of particles and much narrower bandwidth than those of inhomogeneous silver island films. DCM and Rh700 dyes were used to seek for the optimal conditions for the efficient MEF with each SCF. The SCFs with SPR bands overlapped or slightly blue-shifted from the absorption and emission bands of dye molecules, exhibited most efficient fluorescence enhancements. Relative contributions of enlarged electric fields around the nanoparticles and SPCE to the total fluorescence enhancements of DCM and Rh700 were investigated by time-resolved fluorescence spectroscopy (TCSPC and femtosecond transient absorption techniques) and FDTD simulations. The emission of both dyes was found as dominantly increased by the induced local electric fields rather than the plasmon coupled emissions.

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Code: **PHYS.P-119**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Homogeneous gold colloidal surfaces optimal for metal-enhanced fluorescence

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When fluorophores exist in close proximity to plasmonic metal nanoparticles, the fluorescence of dye molecules is strongly enhanced. Exact mechanisms of metal-enhanced fluorescence (MEF) are not yet fully understood, but the locally increased electric field around metal nanoparticles and the plasmon coupled emission of metal nanoparticles have been proposed as those. The MEF shows strong dependence on the properties of the surface plasmon resonance, which is strongly dependent on the size and shape of metal nanoparticles and the metal-fluorophore distance. In this work, the gold colloidal surfaces (GCFs) were synthesized by attaching homogeneous gold colloidal nanoparticles to glass substrates which were prepared by the seeded growth method. The absorption spectrum and the SEM images of GCFs were measured and the GCFs showed high homogeneity in size and the extinction spectra were shifted from visible to near-infrared region depending on the particles size. For the fluorescence enhancement measurements, the GCFs with the 125 nm diameter were found as optimal for the MEF with some NIR dyes. For the study of enhancement mechanisms, time-resolved fluorescence spectroscopy with time-correlated single photon counting system and FDTD simulation were also used.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-120**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Molecular Dynamics Simulation Study of Self-assembled Supramolecular Nanotubule

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In recent experiments, diverse novel supramolecular nanotubules are prepared by adopting non-covalent bonding amphiphiles as the building block to mimic these biological structures. Despite this active experimental studies in preparing various self-assembled nanostructures, the focus is mainly on the achievement of diverse structures with certain geometries: how various interactions cooperatively drive the aggregation, how they optimize and stabilize the self-assembled structure are yet to be explained. To manipulate the size and shape of the assembled structures as we expect, we need to be able to control these interactions through qualitative and quantitative understanding of this process. For the purpose of identifying the exact geometry of self-assembled structure at molecular level and examining the stabilizing interactions and aggregation mechanism, molecular dynamics simulation can be a very useful tool. We performed molecular dynamics simulation on self-assembled supramolecular nanotubule constructed by bent-shaped rod amphiphile as a building block. By systematically examining from small aggregate composed of several molecules to fully constructed toroidal shape, we identified optimal structure consistent with experimental data. Energetic analyses are performed to figure out how cooperative contribution of various interactions select and stabilize the optimal structure. These interactions also play a role as a driving force to construct a nanotubule from small fragmental intermediates. Potential of mean force calculation could provide the mechanism of this assembly process. Our results suggest how molecular dynamics simulation could provide useful insights on principles governing the formation of such structures.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-121**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Effect of Nanoparticles on the Stabilization of a Polymer Nanofiber

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Although polymer nanofibers are considered promising materials due to remarkable stiffness and tensile strength, the instability of the polymer nanofibers is an obstacle to many applications. Recent studies¹ showed that when the polymer nanofiber was made of both polymers and nanoparticles (NPs), the stability was enhanced. It remains, however, unanswered how the NPs in the nanofiber could enhance the stability. In this work, we perform molecular dynamic simulations for a polymer nanofiber with NPs and measure the breakup time of the fiber (i.e., how long the nanofiber stays stable before being disrupted). We find that the introduction of NPs into a fiber increases the breakup time of the fiber significantly. We also find that the spatial arrangement of NPs in the fiber depends on the interaction between NPs and polymers: NPs are located at the center (or surface) when the interaction between NPs and polymers is attractive (or repulsive). The spatial arrangement of NPs and attraction between NPs and polymers affect surface tension and viscosity of the fiber, which in turn affect the stability of the polymer nanofiber. Our simulation results are consistent with previous results from continuum mechanics².

[1] Jeong, J.S. et al., Mechanical properties of electrospun PVA/MWNTs composite nanofibers. *Thin Solid Films* 515 5136 (2007)

[2] Tomotika, S., Instability of a thread of viscous liquid. *Proc. R. Soc. London, Ser. A* 150 322 (1935)

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-122**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Infrared multiphoton dissociation of a-type peptide ion derived from triglycine by experiment and theory

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Peptide ions isomerize while undergoing fragmentation in the gas phase. To address this issue, we studied the unimolecular dissociation of the a-type ion derived from protonated triglycine. We calculated the microcanonical rate constant for every step of isomerization using the RRKM theory based on ab initio potential energy surface. We also obtained the infrared multiphoton dissociation (IRMPD) spectra of the a-type ion by experiment. The overall reaction rate is numerically simulated to examine the temporal variation of the isomers of the a-type ion prior to dissociation as a function of internal energy. Comparison of the calculated infrared spectra with experiment suggests that resulting infrared spectra are determined by the population of the transient isomeric species. Thus, the infrared spectra of peptide ion result from the reaction intermediates involved in unimolecular dissociation rather than the reactant ion.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-123**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Oxygen/Water Redox Couple Modulating Interfacial Charge Transfer of Graphene

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Low dimensional carbon materials in the ambient conditions undergo spontaneous hole doping, the detailed mechanism of which has yet to be revealed. In this work, we propose a mechanism based on a redox couple of O_2/H_2O and verify it for two model systems: i) annealing-induced charge transfer of graphene/ SiO_2 in air and ii) acid-induced charge transfer of graphene/ SiO_2 in water. Raman spectroscopy and water contact angle measurements were used to quantify the charge density in graphene and hydrophilicity of substrates, respectively. First, thermal annealing enhances the degree of the charge transfer in silica-supported graphene exposed to oxygen and water vapor. Mechanically exfoliated graphene samples on silicon dioxide substrates were annealed at various temperatures in a range of 100 ~ 1000 °C to induce the hole doping. While the annealing-induced charge density of graphene increased with increasing annealing temperature up to 700 °C, it decreased as increasing the temperature further higher. Water contact angle measurements showed that the charge transfer rate is proportional to the hydrophilicity of the substrates. Graphene samples prepared in a low humidity condition lead to significantly decreased charge transfer suggesting that water contained between graphene and substrate plays a key role. For the second system, we found that graphene in acidic solution is hole-doped and the responsible charge transfer requires dissolved oxygen. The proposed mechanism will be discussed to explain the experimental results observed for the two model systems.

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Code: **PHYS.P-124**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

IR probing of equilibria between I₂ and SCN⁻ in DMSO

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I₂ reacts with SCN⁻ producing ISCN and I₃⁻ in solutions. In this work, we investigated the equilibrium between I₂ and SCN⁻ by using Raman, FTIR, UV-Vis, IR pump probe (IR PP), and 2-dimensional infrared (2DIR) spectroscopy. We demonstrated that thiocyanate induces a disproportional reaction of iodine ($2\text{I}_2 + \text{SCN}^- \rightarrow \text{ISCN} + \text{I}_3^-$) in various solvents such as methylene chloride, ethanol, ethyl acetate, and DMSO. The disproportional reaction of iodine in DMSO is studied by probing the CN stretch vibrations of thiocyanate. The vibrational and orientation relaxation dynamics of ISCN and SCN⁻ are studied by IR PP spectroscopy and the forward and backward reaction rates are determined by 2DIR spectroscopy. The disproportional equilibrium of iodine in DMSO is found to occur on hundred picosecond timescales.

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Code: **PHYS.P-125**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Completing the Picture of Quinophthalone Photochemistry

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Although the highly unusual case of excited state intramolecular proton transfer (ESIPT) of quinophthalone (QPH) has recently been reported in some detail, the relaxation pathway to the ground state after the ESIPT remains elusive to date. Moreover, the fact that the excited-state lifetimes and spectral bands are not fully explained indicates that additional states and/or processes may be involved in its excited state dynamics. In order to map out the complete picture for the complex photophysics of QPH, we conducted various spectroscopic experiments including ultrafast time-resolved transient absorption spectroscopy in different reaction environments.

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Code: **PHYS.P-126**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Noble metal-free MOF-derived onion slice-type hollow cobalt sulfide nanostructures: Enhanced activity of CdS for improving photocatalytic hydrogen production

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The Hollow materials have played a significant role in cutting-edge innovations for energy conversion due to their peculiar properties and their wide range of potential applications. These materials show great promise for the development of cleaner power sources to address growing environmental concerns at a time of increasing global demand for energy. Noble metal-free MOF-derived onion slice-type hollow structured Co_4S_3 was developed and embedded with CdS nanoparticles for photocatalytic hydrogen production. The incorporation of Co_4S_3 with the CdS particles effectively accelerated charge separation and transfer in photocatalytic reactions due to the low density, hollow interior, and shell permeability of the onion-type composite. The optimized $\text{Co}_4\text{S}_3/\text{CdS}$ photocatalyst led to an enhanced rate of H_2 production of $12,360 \mu\text{mol}\cdot\text{h}^{-1}\cdot\text{g}^{-1}$ under simulated solar light irradiation; this value is 26-fold greater than that of the pristine CdS nanoparticles. The $\text{Co}_4\text{S}_3/\text{CdS}$ composite exhibited remarkably stable photocatalytic performance for up to 65 h and could be reused in five successive cycles. Furthermore, to the best of our knowledge, this is the highest H_2 production rate achieved with cobalt sulfide-based CdS nanoparticle photocatalysts in the photocatalysis of water under simulated solar light irradiation. Owing to its low cost and high efficiency, this photocatalytic system should hold great potential for the development of highly efficient photocatalytic materials for use in various fields.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-127**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Excited-state Dynamics of Resveratrone and Its Interaction with DNA

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Resveratrone is a highly fluorescent organic compound photochemically derived from resveratrol, one of phytoalexins abundant in nuts, berries, and grapes. It has many desirable traits as a versatile fluorophore, including a large Stokes' shift, high fluorescence quantum yield, and large two-photon absorption cross-section. We studied properties of this novel molecule with various steady-state and time-resolved spectroscopic techniques in pursuit of detailing its excited-state dynamics and unraveling the origin of its unique properties. In particular, we found that the molecule interacts significantly with DNA, changing its absorption coefficients and photoluminescence quantum yield. The effect of this interaction on the dynamics of resveratrone was investigated.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-128**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

ER Recombination Dynamics of Gas-phase Nitrogen Atom Reaction with Chemisorbed Nitrogen Atoms on a W(100)

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We have calculated the probability of N₂ formation and energy deposit of the reaction exothermicity in the newly formed N₂, particularly in its vibrational motion, in the gas-phase reactions N(g) + N(ad)/W → N₂(g) + W. The reaction probabilities are about 0.01 at gas temperature 1800 K and surface temperature 300 K. The vibrational and translational motions of product N₂ share most of the reaction energy. Increasing the initial vibrational state of the adsorbate from the ground state to v = 1, 2 and 3 causes the energies shared by product vary only slightly. The product vibrational excitation in N₂ is strong, leading to a population inversion. The amount of energy propagated into the bulk solid phase is negative, which means the energy transfer from the surface to the desorbed product. The dependence of reaction probabilities and energy distributions on surface temperature is found to be weak, in the range of 0 – 1500 K.

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Code: **PHYS.P-129**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Multidirectional-charge-transfer urchin-type Mo-doped $W_{18}O_{1849}$ nanostructures on CdS nanorods for enhanced photocatalytic hydrogen evolution

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Transition metal oxides (TMOs) have attracted considerable attention because they provide eco-friendly ways of collecting solar energy and are more stable than sulfides or phosphides for photoirradiation over long periods without photocorrosion. Among TMOs, tungsten oxides have attracted considerable attention in the field of photocatalysis owing to their excellent electron transport properties and good resilience to photocorrosion in aqueous media. However, pristine WO_3 exhibits low photocatalytic activity because of rapid recombination of photogenerated charge carriers and its narrow photoabsorption range. Consequently, the monoclinic oxygen-deficient ($WO_{3-\delta}$) material $W_{18}O_{1849}$ ($\cong WO_{2.73}$) has attracted significantly greater interest than simple tungsten oxides owing to its high chemical stability and large number of oxygen vacancies (OVs). In particular, the water splitting efficiency of $W_{18}O_{1849}$ is enhanced by doping with Mo, which modifies the intrinsic chemical properties of $W_{18}O_{1849}$ without disturbing its crystal structure, while producing more active sites. Furthermore, by tuning the morphology of Mo- $W_{18}O_{1849}$ (MWO) the photocatalytic activity of MWO-embedded CdS greatly enhanced by its exposed high surface area and supplementary active sites. To that end, we developed an urchin-type MWO cocatalyst integrated into a CdS nanorod (NR) by simple methods; this catalyst exhibits an enhanced rate of H_2 production under simulated solar light irradiation of $\sim 40,225 \mu\text{mol h}^{-1} \text{g}^{-1}$, which is 20 times higher than that of pristine CdS. The urchin-type morphology significantly shortens charge-carrier transport distances. The oxygen deficiency and Mo dopant in the $W_{18}O_{1849}$ system greatly improves the number of active sites, in turn promoting the efficient utilization of light, excellent electron-transport properties, and good resilience to photocorrosion. These properties are especially beneficial for effective excitation and the separation of charge carriers that are then directed to the reduction of protons

to H₂. Moreover, to the best of our knowledge, this material exhibits the best performance among reported tungsten-based oxides as a cocatalyst on CdS-composites.



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Area: Physical Chemistry

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Computational study on a highly-ordered hydroxylated graphene epitaxially-grown on Cu(111)

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Graphene functionalization is of great importance in applying graphene as a component in functional devices or in activating it for use as a catalyst. Here we investigate the formation mechanism of highly-ordered hydroxylated graphene (OH-Gr) epitaxially-grown on Cu(111) substrate using periodic density functional theory (DFT) calculations. The OH-Gr with $(\sqrt{3}\times\sqrt{3})R30^\circ$ superstructure observed in scanning tunneling microscopy (STM) experiment is thermodynamically more stable and also has a lower activation energy than other ordered configurations. We revealed a feasibility of graphene enolate plays a key role in the formation of highly-ordered OH-Gr, which can be formed with removing the hydrogen atom from a hydroxyl group adsorbed on a graphene by a secondly approaching hydroxyl species. Our previous computational study suggested that improved interfacial interaction between graphene and the metal substrate makes the graphene enolate a local minimum and further highly stabilizes it over the graphene epoxide.^[1] Therefore, the further hydroxylation can be proceeded without termination due to the formation of graphene epoxide. Our results provide not only a novel perspective for a chemical route to functionalizing graphene but also a new opportunity to utilize highly-ordered OH-Gr for graphene-based applications.

[1] J. Jung, H. Lim, J. Oh, and Y. Kim, *J. Am. Chem. Soc.* 136, 8528 (2014).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-131**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Effect of Surface Functionalized Multi Walled Carbon Nanotubes as Light Harvesting Material to CdS Nanorods for Effective Photocatalytic Water Splitting Hydrogen Generation

MADHUSUDANA GOPANNAGARI, Hanbit Park, EunHwa Kim, Amaranatha reddy, TaeKyu Kim*

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Photocatalytic H₂ production from water splitting is of promising potential to resolve the energy shortage and environmental concerns. During the past decade, carbon materials have shown great ability to enhance the photocatalytic H₂ production performance of semiconductor photocatalysts. Decorating CNTs with photoactive materials has received great attention for solar light conversion in energy and environmental fields. This study reports the influence of carboxylic, sulfonic, amine, ascorbic acid functional groups and metal nanoparticles tethered to the CNTs and this system to the CdS photocatalyst. Among these functional groups, ascorbic acid functionalized (Af-CNTs) decorated on CdS nanorods six times improved the photocatalytic H₂ production than CdS. However, Pt nanoparticles as cocatalyst in the binary nanohybrids between Af-CNT and CdS 47 fold than CdS and seven times than Af-CNT/CdS enhanced. The Pt-Af-CNT on CdS showed higher in amount of H₂ production due to surface electron hole separation is high and low recombination rate. The functional groups on CNTs play a crucial role in determining the charge transfer direction, active sites for reduction reactions in water. This results were compared with primary carboxyl functionalized CNT(Pt-Cf-CNT/CdS) and photocurrent measurements also indicated that Pt-Af-CNT/CdS ternary generates a higher photocurrent than that of Af-CNT/CdS binary (ternary>binary>CdS alone) and Pt-Cf-CNT/CdS nanohybrids. The photocatalytic performances of such hybrids for H₂ production were found to be highly influenced by surface states of CNT suggesting the importance of surface treatment of CNTs. Detailed surface studies were also described using XPS, Raman spectroscopy, FTIR, XRD, TEM.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-132**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electromagnetic coupling in graphone/In₂Se₃ nanocomposite

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Electron spin has been used mainly as data storage application and also possesses great potential as futuristic spintronic devices and spin qubits. However, manipulating electron spins by applying a magnetic field requires a large power, thus electrical control of magnetism is of great technological and scientific interest. Compounds exhibiting such magnetic response to an applied electric field are very rare and the coupling strength is too weak. For realistic applications, an artificial composite system composed of ferromagnetic and ferroelectric materials has been one of attempts, and recently a significant attention has been paid to nano-composite materials. Here a nanocomposite material composed of light-weighted ferromagnetic material, graphone, and a monolayer ferroelectric material In₂Se₃ is studied. The electromagnetic coupling strength is calculated by using the density functional theory method and its perspective is discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-133**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A study on photophysical properties of PANI composites free standing films

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Department of Chemistry, Sahmyook University, Korea

¹*Division of General Studies, Sahmyook University, Korea*

PANI (poly aniline) as one of the conducting polymers has widely been used in the wide range of applications due to distinctive redox properties, superior stability to air oxidation, and an ease of synthesis. The electrical properties of PANI can be influenced by degree of polymerization, percentage of crystallinity, oxidation state level by doping ratio, and type of dopant. In this study, we prepared free standing films based on PANI composites for studying photo-physical properties. The PANI was synthesized by using emulsion polymerization method from aniline with different acid doping degree. Morphology, electrical properties, and photo-response of the PANI composites were investigated.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-134**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Preparation of TiO₂/ZrO₂ composites for hard and transparent coating

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¹*Division of General Studies, Sahmyook University, Korea*

Titanium oxide (TiO₂) and zirconium oxides (ZrO₂) are one of the most studied ceramic materials used in the wide range of application because of their remarkable mechanical, thermal and chemical properties. In the recent years, film forms of both materials have been broadly studied in antireflective and protective coating, optical coating, and insulating films for field effect transistors due to its high dielectric constant, high refractive index, and transparency in the visible spectral range. In this study, we prepared TiO₂, ZrO₂ and TiO₂-ZrO₂ composites film deposited by sol-gel process for hard coating applications. We characterized the structural properties and chemical composition of coating material with XRD, XPS and FT-IR, and optical property was carried out by using UV-vis spectroscopy. We confirmed mechanical property by using various hardness-testing methods.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-135**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Self-regulation under intracellular noise

Hoongi Lee, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

Cells are noisy biochemical reactors: low reactant numbers can lead to significant statistical fluctuations in molecule numbers and reaction rates. Some analytical framework describing the steady-state protein concentration in living cells have been suggested and they revealed that noise is essentially determined at the translational level, and that the mean and variance of protein concentration can be controlled independently. However, changes in environmental conditions lead to expression variation that manifest at the level of gene regulatory networks. For quantitative understanding of probabilistic behaviors of living cells, it is essential to construct a correct mathematical description of intracellular networks interacting with complex cell environments. By applying the present approach to the gene expression network, we obtain simple analytic results for the gene expression variability and the environment-induced correlations at the translational level.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-136**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Formation and Structure of 1-Adamantyl Isocyanide Self-Assembled Monolayers on Au(111)

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Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are organic assemblies spontaneously formed on surfaces by adsorption of molecular constituents. The formation and structure of 1-adamantyl isocyanide SAMs on Au(111) prepared by solution deposition methods have been investigated by scanning tunneling microscopy (STM) and cyclic voltammetry (CV). STM imaging revealed that the surface structures of 1-adamantyl isocyanide SAMs prepared by solution deposition method are noticeably different from 1-adamantanethiol SAMs, the most extensively studied class of SAMs. Even though both SAMs have same adamantyl functional group, 1-adamantyl isocyanide SAMs showed less ordered structure compared to 1-adamantanethiol SAMs. CV measurements showed that reductive desorption peak for 1-adamantyl isocyanide SAMs was observed at around -850 mV, whereas that for 1-adamantanethiol SAMs was observed at around -1000 mV. This result means NC-Au interaction for 1-adamantyl isocyanide SAMs is weaker than the S-Au interaction for 1-adamantanethiol SAMs. By comparing two different SAMs, we found that 2-D surface structures of 1-adamantyl isocyanide SAMs are highly influenced by active headgroup.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-137**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A theoretical study on the singlet-triplet energy difference of gold-containing organo-metallic complexes

CHANGHWAN AHN, Dongwook Kim^{*}

Department of Chemistry, Kyonggi University, Korea

Organic Light Emitting Diodes (OLEDs) promise highly efficient lighting and display technologies. However, to obtain high efficiency OLEDs, the energy gap between singlet and triplet states must be small. Recently, there have been studies to adjust the energy gap between singlet and triplet states using gold-containing organo-metallic complexes. In this study, we investigated the electronic structure change according to dihedral angle (0-90°) used gold carbene-metal-amides (CMA1) to elucidate the photophysical properties of gold-containing organo-metallic complexes and calculated that how the energy gap between singlet and triplet is affected. To understand the link between molecular geometry and the energetic ordering of singlet and triplet states, the energies and optimized molecular structures of the ground (S0), first excited singlet (S1) and triplet (T1) states for CMA1 were calculated using DFT and time-dependent DFT (TD-DFT).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-138**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Theoretical Study on Dicyanobenzene Organic Light Emitting Diode Material: Calculation result of position of carbazole and DMAC

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Department of Chemistry, Kyonggi University, Korea

Recently, Thermally Activated Delayed Fluorescence (TADF) has been widely utilized to fabricate highly efficient OLEDs. In order to facilitate TADF, a small value of ΔE_{ST} is required. To this end, TADF molecules should have spatially separate HOMO and LUMO within electron-donor and acceptor groups, respectively. In this sense, the torsional angle between the donor and acceptor subunits has been proposed as a factor to consider. Therefore, in this study, we investigated the effect of such a torsional angle on ΔE_{ST} . We employed Carbazole and 9,9 - dimethyl - 9,10 - dihydroacridine (DMAC) as electron donating groups, and dicyanobenzene as an electron accepting unit. Electronic structures of such molecules were calculated at Density Functional Theory level using gap-tuned WB97X functional and 6-31G(d) basis sets.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-139**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Structural comparison with PDGFRA mutations in GIST: Molecular dynamics simulation

Cheol hee Kim, Eunae Kim*

Department of Pharmacy, Chosun University, Korea

Gastrointestinal stromal tumor (GIST) is the most common gastrointestinal tumors in the development of gastrointestinal stroma, with the potential for malignant tumors. GIST is caused by mutations in the KIT or Platelet-Derived Growth Factor Receptor-alpha (PDGFRA) belonging to the Receptor Tyrosine Kinase (RTK) type III. Approximately 85% of the GIST mutations were observed in the KIT gene and 10% of the GIST mutated in the PDGFRA gene. Until 2002 year, the surgical therapy of GIST had a poor prognosis and favorable tumor drugs didn't exist. Recently, imatinib has been developed and the imatinib treatment of GIST is good well when the surgical treatment is not possible or the tumors spread to other organs. However, it has been reported that KIT and PDGFRA are resistant to imatinib due to mutations in the activation-loop (A-loop) site. Therefore, the development of new drug has been still required. In this study, we focused that D842V mutant such as the A-loop mutant of PDGFRA was resistant to imatinib and the D842Y mutant was higher in the activation of imatinib. We try to predict the structures of two mutants using molecular dynamics simulation (MD). Based on the X-ray structure of wild-type PDGFRA (PDB ID: 5K5X), the structures of D842V and D842Y PDGFRA are constructed and are fully equilibrated in aqueous solution of temperature 310 K and pressure 1 atm. The MD trajectories of D842V, D852Y mutants and wild-type are analyzed to compare the atomistic features of the mutant structures corresponding to the amino acid effect of A-loop and additionally the binding pose of imatinib depending on the mutation receptors.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-140**

Area: Physical Chemistry

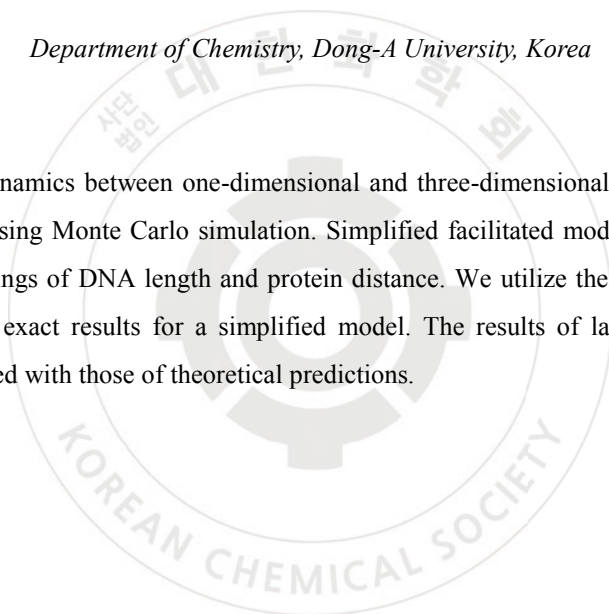
Type: Poster Presentation, Time: FRI 13:00~14:30

Facilitated Protein-DNA binding reaction with Monte Carlo simulation : DNA length and protein distance

junmyeong jeong, Taejun Kim^{*}, Hyojoon Kim^{*}

Department of Chemistry, Dong-A University, Korea

We study correlated dynamics between one-dimensional and three-dimensional diffusive movements of DNA-protein binding using Monte Carlo simulation. Simplified facilitated modeling and controlling are studied for various settings of DNA length and protein distance. We utilize the simulation methods that can provide numerical exact results for a simplified model. The results of lattice-based Monte Carlo simulations are compared with those of theoretical predictions.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-141**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Study of Comparison of DFT and DFT-D Method

Youjin Kim, Dongwook Kim*

Department of Chemistry, Kyonggi University, Korea

Density functional theory (DFT) calculation is a type of electronic structure calculation that is the most widely used method. The present study was conducted to investigate the difference between dispersion corrected DFT calculations and DFT calculations without dispersion correction and to find a more accurate calculation method. Both calculations were performed on three types of benzene dimers, T-shape, face-to-face eclipsed(F2F-E) and face-to-face staggered(F2F-S) in lowest singlet (S_1) and triplet (T_1) excited states. Potential energy curves along the distance of benzene dimer are examined by density functional methods B3LYP, PBE0, wB97X, CAM-B3LYP and dispersion corrected methods B3LYP-D3, PBE0-D3, wB97X-D, CAM-B3LYP-D3, with basis sets 6-311++G**. Additional EOM-CCSD calculations were used as reference data.

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Code: **PHYS.P-142**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

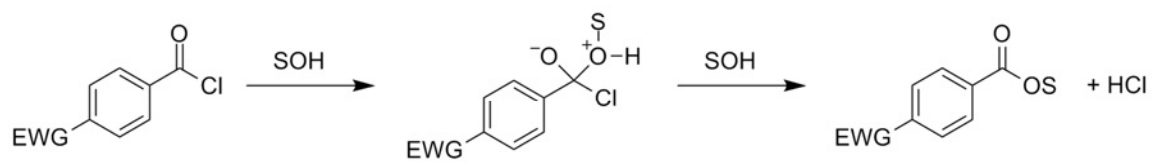
The Kinetical Effect of 4-Fluorosulfony substituent for the Solvolysis of Benzoyl Chloride

JUNGEUN KIM, Kyoung-Ho Park*

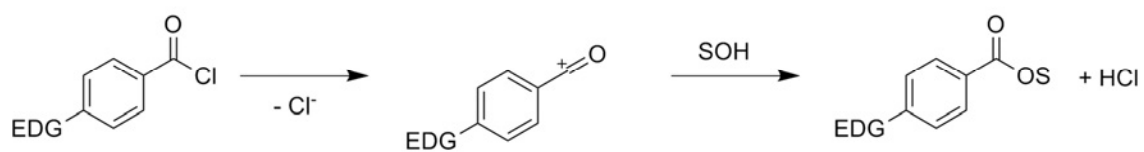
Department of Chemical Molecule Engineering, Hanyang University, Korea

The kinetical results of 4-(fluorosulfonyl)benzoyl chloride was obtained in typical solvolysis conditions, 25.0 °C, pure and binary solvents with water, and by the conductivity method. There were the simple and extended Grunwald-Winstein equations, activation parameters, and the kinetic solvent isotope effect (KSIE) used for analyzing the mechanism. The reaction aspects were compared with previously reported other derivatives in order to confirm the results in detail. 4-(Fluorosulfonyl)benzoyl chloride has a fluorosulfonyl group at *para*-position of benzoyl chloride. In general the fluorosulfonyl group is expected that it could pull the electrons from benzene ring by inductive effect, because the substituent is consist of many strong electronegative atoms, while it could have a resonance effect. This group is located without a steric hindrance, and this location is best place for the inductive and resonance effects on benzene ring. Considering these reasons, the solvolysis of 4-(fluorosulfonyl)benzoyl chloride was expected the unimolecular pathway for solvolysis due to the stronger resonance effect than the inductive one. The results of 4-(fluorosulfonyl)benzoyl chloride were also compared with 4-methoxybenzoyl chloride and 4-(trifluoromethoxy)benzoyl chloride which were previously reported that they have the unimolecular (ionization) pathway.

1. Bimolecular Pathway



2. Unimolecular Pathway



Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: **PHYS.P-143**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Kinetical Phenomenon of 3-(Trifluoromethoxy)benzoyl Chloride in Solvolysis

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The solvolysis of 3-(trifluoromethoxy)benzoyl chloride was studied in usual reaction conditions, 25.0 °C, pure and binary solvents with water, and the conductivity method. The kinetical phenomenon of 3-(trifluoromethoxy)benzoyl chloride was revealed by simple and extended Grunwald-Winstein equations, activation parameters, and the kinetic solvent isotope effect (KSIE). Additionally, the results were compared with previously reported other benzoyl chlorides for confirming the reaction mechanism. 3-(Trifluoromethoxy)benzoyl chloride has a trifluoromethoxy substituent at *meta*-position of benzoyl chloride system. This substituent is located without a steric hindrance, however, it has the effect to pull the electrons from benzene ring due to three fluorine atoms on methoxy group, and also it is possible to have a resonance effect. Therefore the solvolysis of 3-(trifluoromethoxy)benzoyl chloride was expected that the different aspect with 4-(trifluoromethoxy)benzoyl chloride which is already reported by our group. Because the *meta*-position is not convenient to make the resonance effect to benzene ring. Combining all results and the comparison with previously reported derivatives, it was resulted that the mechanism of 3-(trifluoromethoxy)benzoyl chloride undergo through unimolecular(ionization) pathway, but the strength of inductive effect of 3-trifluoromethoxy group was a little weaker than 4-trifluoromethoxy group.

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Code: **PHYS.P-144**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Chemical Fluctuation: beyond the Poissonian paradigm

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The generality of the Poisson process has led to its utilization by researchers in the field of reaction kinetics, and there is numerous research constrained to the Poissonian paradigm. The quantitative analysis of kinetics has started to expand beyond this Poissonian paradigm, however, all research on topic has assumed that either the creation or annihilation process is still Poissonian in nature. In general, however, it is possible that both creation and annihilation process are non-Poisson processes, and this case has recently been reported in biochemical reactions in the living cells. For example, mRNA in the eukaryotic system is created with fluctuating rate and begins to degrade only after the polyadenylate tails are consumed, which is a multi-step degradation process and, therefore, can only be a non-Poisson process. Here, without Poissonian restrictions in both the creation and annihilation processes, we propose a quantitative method to calculate the time correlation function of the product concentration and analyze the power spectrum, the measure of chemical fluctuations. We verified the analytic result through the simulation considering an example where the product is created and annihilated both catalyzed by enzymes but by different ones. We show how the creation rate correlation and non-Poissonity of annihilation process contribute to the chemical fluctuations.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-145**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Collective Cell Division Model for Estimating Stochasticity in Cell Lineage

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The division of a single cell is often asymmetric and stochastic: (1) the distributions of the cellular components of two daughter cells are not equal after the division and (2) the concentration of protein determinants in daughter cells are seemingly stochastic. Due to such asymmetric and stochastic cell division, daughter cells may face totally different fates, thus sometimes developing into cancer. Therefore, it is an issue of practical importance but remains a formidable task to estimate how stochastic the cell division of a given type of cells would be. In this work, we develop a model for the cell division based on stochastic differential equations and compare the model to the experiments for HeLa cell. We employ fluorescent ubiquitination-based cell cycle indicator (Fucci) that marks G1 and S/G2/M phases with red and green colors, respectively. Then, we estimate the number of cells in red and green phases over generations of cells. If the cell were to be non-stochastic, all cells would have the same cell cycle and the ratios of red and green cells would keep oscillating. Interesting is that the ratios of red and green cells stop oscillating after a few generations. Our model consists of two stochastic differential equations with a set of parameters obtained from previous studies (synthesis and degradation rates of protein, hill coefficient, and dissociation constants). By adjusting the stochasticity in the equations, we tune the heterogeneity of cell division and reproduce the experimental results successfully. The method used in this work bridges individual cell's property and their collective behavior, and provides a systematic way of estimating the stochasticity. This approach is also noteworthy since we do not encounter cells individually, but en masse.

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Code: **PHYS.P-146**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Molecular Engineering of Spirofluorene-dithiophene based Hole Transport Materials for Perovskite Solar Cell

Maebienne Anjelica Gapol, Sang Hee Lee, Dong Hee Kim *

Department of Chemistry, Kunsan National University, Korea

Various studies have been dedicated to the development of perovskite solar cell (PeSC) which has a high certified power conversion efficiency of 22.1%. Discovery of a cheaper and more efficient hole transport material (HTM) for PeSC have been an active area of research. In this presentation, we designed HTMs based on spirofluorene-dithiophene having two diphenylamine arms. Different substituents were attached to the phenyl group of the core moiety to elucidate the roles of various outer substituents on the physical properties of the HTM. Energy levels, absorption spectra and electrochemical properties of the derivatives were investigated using the density functional theory and time-dependent density functional theory.

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Code: **PHYS.P-147**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Theoretical Insights on Perylene-Based Dyes for Solar Cell Application

Liezel Estrella, Sang Hee Lee, Dong Hee Kim *

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Computational chemistry has been very valuable in the field of solar energy harvesting. In dye-sensitized solar cell (DSSC) for instance, a strategic approach is the molecular engineering of dye sensitizer using reliable and inexpensive computational methods prior to the synthesis of the dyes. In the research presented herein, novel perylene-based dyes were systematically designed for possible applications in dye-sensitized solar cells. Density functional theory (DFT) and Time-dependent DFT methodologies were employed to investigate the key properties of the dye sensitizers that are necessary to properly understand the primary role of the dyes in the photon-to-electricity conversion in a solar cell device. Various parameters including the geometry, absorption spectra, oxidation potential, and electronic structure, were assessed to fully comprehend the structure property relationships of each design. These theoretical results may serve as a potential reference for the future dye designs for DSSC applications.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-148**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Cationic effects on the Excited-State Proton Transfer Reaction of a Photoacid in Aqueous Solutions

Joonyoung F. Joung, SangIn Kim, Sunnam Park*

Department of Chemistry, Korea University, Korea

Proton transfer (PT) reaction in aqueous ionic solutions is highly affected by dissolved ions. However, the role of ions in PT has not been understood on a molecular level. In this study, excited-state proton transfer (ESPT) reactions of a photoacid (Coumarin 183, C183) in aqueous metal chloride solutions were systematically investigated by using time-resolved fluorescence spectroscopy and quantum chemical calculation. As the charge density of cations increases, the activation energy for the ESPT reaction of C183 is shown to be increased. Furthermore, the hydrogen bond length between C183 and water molecule in the first cationic hydration shell is highly correlated with both the activation energy and the charge density. In the transition state (TS), the positive charge of proton is delocalized along the hydrogen-bonded water channel. The TS is highly destabilized by the cations. For the first time, we were able to successfully elucidate the underlying mechanism of the cationic effects on the proton dissociation reaction of a weak acid and subsequent PT process in aqueous metal chloride solutions.

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Code: **PHYS.P-149**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Characterization of Mixed Zn(II)/Gd(III) Oxide Nanoparticle T₁ MRI Contrasting Agent

tirusew tegafaw, Gang Ho Lee^{*}

Department of Chemistry, Kyungpook National University, Korea

D-glucuronic acid coated mixed Zn(II)/Gd(III) oxide nanoparticles with d_{avg} of 2.1 nm were synthesized. The D-glucuronic acid coated Zn(II)/Gd(III) oxide nanoparticles showed a longitudinal water proton relaxivity (r_1) of $12.3 \text{ s}^{-1}\text{mM}^{-1}$ with $r_2/r_1 = 1.1$, suggesting that the sample suspension will be a good T₁ MRI contrast agent. We attribute this to reduced magnetization of the mixed nanoparticles owing to non-magnetic Zn in the nanoparticles. We characterized particle diameter, hydrodynamic diameter, surface coating, magnetic properties, cellular cytotoxicity, water proton relaxivities, and in vivo T₁ MR images. Highly positive contrast enhancements were observed in T₁ MR images of a mouse.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-150**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Polarization dependence of metal-induced fluorescence of quantum dots on patterned Ag substrate

WonGeun Yang, Weon-Sik Chae *

Daegu Center, Korea Basic Science Institute, Korea

Electronic transition of fluorophores is significantly changed near plasmonic metal surface. As light irradiates on noble metal surface, collective oscillation of free electron reinforces electromagnetic field density near metal surface, which changes absorption and emission transitions of fluorophores. In this study, we performed metal-enhanced fluorescence (MEF) behavior of semiconductor quantum dots (QDs) near patterned plasmonic metal (Ag) substrates. In particular, we studied polarization dependence of emission and MEF enhancement factor near metal nanosubstrates in single molecule level using steady-state and time-resolved fluorescence polarization microscopy. Antibunching experiment presents unique characteristics of single QD emission.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-151**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

MoS₂ Basal Planes Enhances Electrochemical Hydrogen Evolution Reaction: First-Principles Study

MIN CHOI, Hyun Woo Kim, Youngmin Kim¹, Hyung Ju Kim¹, Hyunju Chang^{*}

Chemical Simulation Center, Korea Research Institute of Chemical Technology, Korea

¹*Carbon Resources Institute, Korea Research Institute of Chemical Technology, Korea*

Molybdenum disulfide (MoS₂) is considered as a promising catalyst which can potentially replace platinum catalysts in electrochemical hydrogen evolution reaction (HER). As MoS₂ has catalytically active edge sites and rather inactive basal planes, activating its basal plane is important to further enhance the HER performance. It was experimentally demonstrated for the first time that electrochemically activated MoS₂ basal planes can improve the HER performance compared to commercial bulk MoS₂. In this study, we modeled MoS₂ monolayer with different curvatures to describe the locally distorted MoS₂ basal plane in this electrochemical activation process. We also calculated hydrogen-binding strengths to the MoS₂ surfaces to explain the enhanced catalytic activity of the distorted MoS₂ basal planes. We found out that the hydrogen atom prefers to bind to more distorted MoS₂ monolayer. As hydrogen-binding can be a descriptor for the HER performance, our computational results indicate activated basal planes can dramatically improve the catalytic efficiency of HER.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-152**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Mechanistic study of acetic acid synthesis over Cu-ZSM-5 framework : A QM/MM study

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CO₂ is well-known as a greenhouse gas. Most researchers have been working to reduce its concentration in the atmosphere. At the same time, however, the carbon dioxide is a potentially valuable chemical as a source of one carbon supplier. It can produce carboxylic acids and alcohol that can convert to various useful materials. The simultaneous activation of CH₄ and CO₂ is possible in the presence of some alkali metals on the zeolite framework. In this work, the simultaneous co-activation of methane and carbon dioxide over Cu-ZSM-5 were investigated by theoretical approach. We utilised the 34T cluster model of ZSM-5 zeolite in the calculations. We adopted QM/MM approach which is an advantageous approach for the large sized system because it reduces the computational cost. In our QM treatment of the ZSM-5, an active site includes aluminium and copper atoms. The other atoms assigned as the MM region. In this QM/MM study, we employed the M06-L functional and ReaxFF 6.0 forcefield. All the calculations were performed by using the Materials Studio DMol³ and QMERA codes.

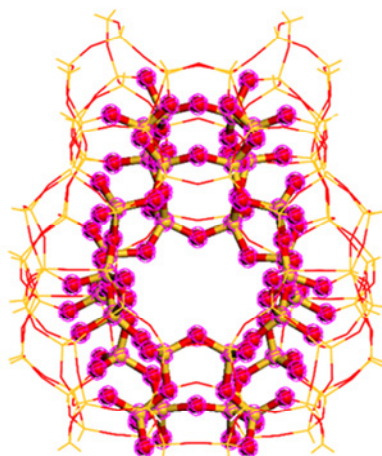


Fig. The optimised structure of the ZSM-5 model. The QM and MM regions are represented in ball-and-stick and a line, respectively.



Conference Date: October 18~20, 2017

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Code: **PHYS.P-153**

Area: Physical Chemistry

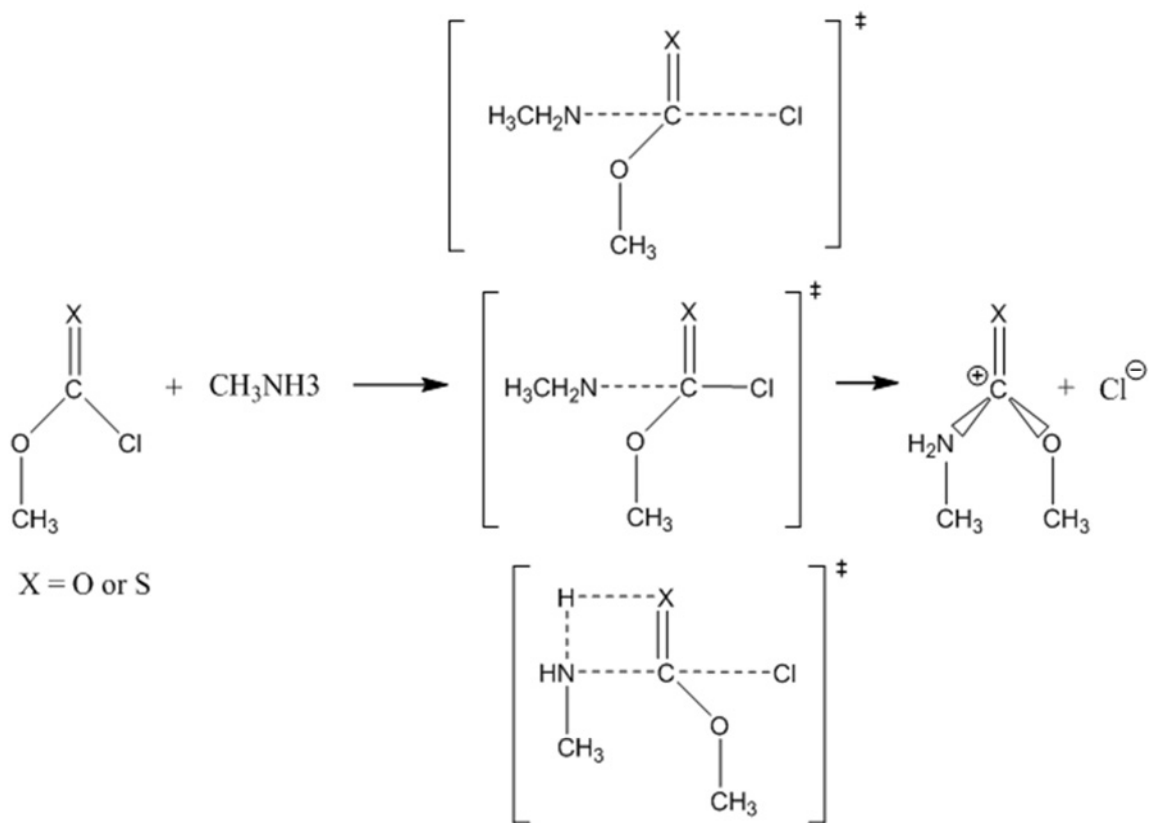
Type: Poster Presentation, Time: FRI 13:00~14:30

DFT Studies on the Aminolysis of Methyl (Thio)Chloro Formates in Acetonitrile

Adhikary Keshab Kumar, Chan Kyung Kim*

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Lots of experimental and theoretical studies have been performed on the aminolysis of carbonyl and thiocarbonyl transfer reactions. The reaction mechanism is still not clear as there are three possible pathways – (1) concerted bimolecular single-step, (2) stepwise addition-elimination, and (3) elimination-addition type mechanisms. Unfortunately, the reaction mechanism involving a planar back-side nucleophilic attack to the leaving group is not possible due to a high energy barrier. To understand the reaction mechanism, we performed DFT calculations at the B3LYP/6-311+G(d,p) level of theory in acetonitrile solvent as the zwitterionic species are formed during the reaction. The calculations show that the concerted nucleophilic attack towards the reaction centre favoured over the stepwise one. The structures and energetics will be discussed in detail.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-154**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Insight into the Universal Descriptor for Heterogeneous Catalysis

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Theoretical calculations are increasingly playing an important role for initial catalysts screening; however, large scale catalysts screening efforts have been stymied by computationally expensive thermodynamics and kinetics calculations. We are in search of some universal descriptors which will be fast and easy to calculate, and can correctly correlate the catalyst activity and selectivity. A promising Pt₃V₅ sub nanometer size cluster was screened from a pool of bimetallic clusters by using Sabatier's principle with Bronsted–Evans–Polanyi (BEP) relation for ultra-low-temperature CO oxidation in hydrogen rich environment by simultaneously tuning of CO and H₂ adsorption strength and water activation over the Pt₃V₅ surface, which could make the hydrogen fuel ultra-pure. The kinetic study confirmed the superiority of Pt₃V₅ over Pt. Using the Sabatier's principle with BEP relations, promising surfaces can be screened but performing all these needs reasonable computational efforts. In this study, we have tried to correlate the adsorption energies with a degree of chemical softness (a descriptor for catalytic activity and selectivity), which is fast and easy to calculate by using the density functional calculations. Finally, we conclude that further insight is needed for the procedure to calculate chemical softness because of poor estimations of energies of so-called virtual orbitals particular for very stable molecules.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-155**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fluctuating Diffusion Kernel: Fickian yet Non-Gaussian Transport in Disordered Media

Sanggeun Song, Ji-Hyun Kim^{*}, Jaeyoung Sung^{*}

Department of Chemistry, Chung-Ang University, Korea

We present a novel formulation to deal with molecular transport process in disordered media, taking into account the non-Poisson waiting time distribution for individual jumps on lattice and its coupling to the environmental dynamics. This approach encompasses the continuous-time random walk (CTRW) capturing transient trapping events and the diffusing diffusivity model accounting for the environmental fluctuation over space or time. On the basis of our formulation, we could identify the diffusion kernel correlation function capturing the multi-scale dynamics of the transport system and provide a practical route to calculate the environmental relaxation time from the first two moments of particle displacement distribution. Comparison between the environmental relaxation time and the diffusion time scale gives a clear and comprehensive explanation on the Fickian yet non-Gaussian diffusion observed from the dense hard-sphere fluid and the supercooled water in molecular dynamics simulations.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-156**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Excited states dynamics of curcumin probe by femtosecond stimulated Raman spectroscopy

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Curcumin has been of great interest to researchers in many disciplines due to its potential applications in antioxidant, anti-inflammatory, and anti-cancer agents. The intramolecular charge transfer (ICT) reaction of curcumin in the excited states has been investigated by time-resolved spectroscopic techniques, but the photophysical properties of curcumin and the solvation dynamics in polar solvents are not clearly understood. The cis-diketo form of curcumin often undergoes a keto-enol rearrangement by transfer of proton from the CH₂ group to form the enol form when it is dissolved in solvent. The ICT reaction product of this cis-enol conformer keeps the same molecular structure as the reactant while the reaction leaves the disruption of the solvation structure behind. In this work, we have investigated the ICT reaction of curcumin and the solvation relaxation of DMSO after the reaction by femtosecond stimulated Raman spectroscopy. The real-time vibrational probe of reactant/product and solvent molecules have provided the enough evidence for the efficient (3-4 ps) ICT process and the following solvation dynamics (15-20 ps) of DMSO.

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Code: **PHYS.P-157**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Disentanglement of DNA Strands Accelerates DNA Ejection Rate

JungBin Park, Bong June Sung*

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Topoisomerase (TOP) is an enzyme that prevents a DNA from being entangled by allowing the DNA strands to cross each other. It has been reported that chain-crossings (which leads to the disentanglement of DNA strands) make the polymer conformational relaxation faster inside the viral capsid. However, scientific questions still remain: whether and how TOP and the disentanglement would affect the ejection of DNA out of the viral capsid, which is an important biological process for viruses. We delineate the importance of maintaining equilibrium conformations during DNA ejection and how chain-crossings play a role in conformational relaxation process. We carry out MD simulations of a single chain with 1024 monomers. By tuning the force constant of FENE (Finitely Extensible Non-linear Elastic) bead-spring model for the chain, we either allow or disallow the chain to undergo chain crossings. In order to investigate the effect of the initial conformation of the DNA on the ejection rate, we employ two types of initial configuration of the DNA; (1) ordered and (2) disordered DNA conformations. We find from our simulations that in case of disordered DNA conformations, the DNA ejection becomes slow by a factor of two or more when the chain crossing is forbidden. TOP and the strand disentanglement help the DNA relax its conformation quite quickly during the ejection process, thus changing the rate of the ejection significantly. We also find that when the DNA conformation is initially ordered, the effect of disentanglement is not significant.

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Code: **PHYS.P-158**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

How to consider fluctuating reaction rates with the number of product molecules in an elementary reaction

Seong-jun Park, Jaeyoung Sung*

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We present new chemical kinetics that consider the fluctuating reaction rates with the number of product molecules. Our study is based on newly established Master equation which describes the reaction rates as a function of the number of product molecules and time. It reveals the relation between the reaction rate and the product number fluctuation, which indicates the counting statistics of the number of the product molecules showing Super-Poissonian (Sub-Poissonian) character when reaction rate increases (decreases) with the number of product molecules. Furthermore, we can also figure out how far an elementary reaction process deviates from renewal process during fluctuating reaction rates.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-159**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Layer-by-Layer Electrodeposited Reduced Graphene Oxide-Gold Nanoparticle Films as Efficient Electrocatalysts in CO₂ Reduction

Kyungjun Kim, Yong Jun Lee¹, Seung-Sang Cha¹, Do Yun Park¹, Ik-Soo Shin^{1,*}, Kuan Soo Shin^{1,*}

Department of ICMC Convergence Technology, Soongsil University, Korea

¹*Department of Chemistry, Soongsil University, Korea*

Gold-based nanostructures have been known as promising materials for the selective electrochemical reduction of CO₂ in aqueous conditions. In this work, stable aqueous dispersion of polyethylenimine (PEI)-capped gold nanoparticles (AuNPs) was prepared using PEI as the reductant of HAuCl₄. The resultant positively charged PEI-capped AuNPs in conjunction with negatively charged reduced graphene oxide (rGO) nanosheets were utilized as nanobuilding blocks for sequential layer-by-layer (LbL) self-assembly of well defined (AuNPs/rGO)_n (n=1~8) films in which AuNPs overspread evenly on the 2-dimensional rGO-modified indium tin oxide (ITO) electrode. The successful growth of each multilayer was monitored by the gradual increase of absorbance upon increasing the number of bilayers in UV-vis spectra. The uniform multilayer formation with the well-dispersed of AuNPs after each LbL assembly was confirmed by scanning electron microscopy and dispersive X-ray spectroscopy. Using as-fabricated (AuNPs/rGO)_n-ITO as a working electrode, the efficiency of the electrocatalytic conversion of CO₂ was investigated by cyclic voltammetry and gas chromatography.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-160**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemical properties of Li-ion battery by using in situ Raman analysis

Soo Min Kim, yeonju Park, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

Li-ion batteries are an energy storage device capable of repeated charging and discharging, that is, a secondary battery. But, the problem with lithium-ion batteries is the loss of capacity over the life of the battery and the resulting degradation in performance. Therefore, an appropriate technique for monitoring the electrodes during battery operation is important for understanding the characteristics of lithium ion batteries. Raman spectroscopy is a useful tool to investigate the surface change of cathode materials in the battery in real time. LiFePO₄ is a cathode active material that has recently attracted attention due to its excellent safety and long life. So, we made batteries using LiFePO₄ materials. In this study, we conducted in-situ Raman and electrochemical experiments of LiFePO₄ battery. More information on the results will be provided in this presentation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-161**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Layer-by-Layer Self-Assembly of Palladium Nanoparticle-Reduced Graphene Oxide Nanosheet Films for Electrocatalytic Applications

**Ju Won Kim, Kyungjun Kim¹, In-Hyun Kim, Sung Min Park, Sena Lee, Ik-Soo Shin^{*},
Kuan Soo Shin^{*}**

Department of Chemistry, Soongsil University, Korea

¹*Department of ICMC Convergence Technology, Soongsil University, Korea*

Numerous efforts are being carried out to design new electrocatalysts for direct alcohol fuel cell (DAFC) anodes that do not contain Pt. Within this context, Pd is emerging as an attractive replacement for Pt in DAFCs. The support materials can also interplay with catalytic metals, which influence the catalytic activity. The durability of the catalyst is also greatly dependent on its support. In this work, 4-dimethylaminopyridine (DMAP)-stabilized Pd nanoparticles were prepared from the aqueous phase reduction of Na₂PdCl₄ using NaBH₄ in the presence of DMAP. The resultant positively charged DMAP-stabilized PdNPs as electrocatalysts in conjunction with negatively charged reduced graphene oxide (rGO) nanosheets as support materials were utilized as nanobuilding blocks for sequential layer-by-layer self-assembly of well defined (PdNPs/rGO)_n films in which PdNPs overspread evenly on the 2-dimensional rGO-modified indium tin oxide (ITO) electrode. The electrocatalytic performances of the as-prepared (PdNPs/rGO)_n-ITO electrodes were then evaluated by measuring the rate of methanol electrooxidation under alkaline condition.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-162**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Computational study on the interfacial electronic structures between π -conjugated hydrocarbon molecules on Au(111)

Youngjoon An, Jaehoon Jung*

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Fundamental insights into the formation of van der Waals (vdW) interface between an organic adsorbate and solid surfaces have not yet been fully achieved due to its weak adsorption characters. Recently, the experimental study using atomically-resolved scanning tunneling microscopy (STM) combined with density functional theory (DFT) computation revealed that a π -conjugated hydrocarbon (π -CHC) molecule, dehydrobenzo[12]annulene (DBA), can have a specific adsorption configuration, even on the noble Au surface [1], although most π -conjugated molecules, in general, distributed randomly on noble metal surfaces. Our previous computational study proposed that the orbital interaction between a π -CHC molecule and the Au surface can play a decisive role in constraining adsorption geometry, i.e., horizontal orientation, even in the typical weak vdW adsorption system. Here, we extend our previous result using other π -CHC molecule, triphenylene (TP), in order to provide deeper and wider insight into the formation of interfacial electronic and geometric structures between an isolated π -CHC molecule and Au surface. The detailed changes in the density of states (DOS), the charge transfer, and the work function with approaching the π -CHC molecules onto the Au(111) surfaces were examined using vdW density functional (vdW-DF) calculations. We found that the interfacial electronic structures are formed in a way to maximize the interfacial orbital interaction between a π -CHC molecule and the noble Au surface through a process of interlocking–dragging–splitting, which involves the local splitting of the Au d state due to the electronic coupling with molecular π -state. We believe that our results provide not only deeper insight into the formation mechanism of interfacial electronic and geometric structures in weak adsorption process but also new perspectives to organic electronics using π -CHC molecules on the Au electrodes.

1.J.-H. Kim, J. Jung, K. Tahara, Y. Tobe, Y. Kim, and M. Kawai, J. Chem. Phys. 140, 074709 (2014).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-163**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Determination of organophosphate compounds based on SERS

Joohee Oh, Sila Jin, yeonju Park, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

Organophosphate compounds have been useful in agriculture and military training and have provided many benefits. But nowadays it becomes major environmental pollutants and it is frequently used in terrorism and war. Nerve agents which is one of the phosphorous-containing organic chemicals are affect the nervous system of the human body. Therefore, quick and effective detection of organophosphate compounds have been investigated. Surface-enhanced Raman scattering (SERS) is an ultrasensitive and effective technique for detection as well as provide rich structural information. However organophosphorus materials are difficult to adsorb on the Ag nanoparticles (NPs). In this study, we were synthesis the dimethyl methyl phosphate (DMMP) and hydroquinone to make it easier to adsorb onto Ag NPs. We successfully detected nerve agent simulants using this method by SERS. Details on the result of detection nerve agent simulants using SERS will be discussed in the presentation.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-164**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Identification of various bacteria on the SERS substrate

Sila Jin, Joohee Oh, yeonju Park, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

Bacteria can be beneficial or harmful to humans depending on the species. Therefore, to prevent damages caused by biological attack, fast and accurate determination and identification of bacteria should be performed. Surface-enhanced Raman scattering (SERS) is a powerful technique to detect biological reagent because it provides rapid and ultrasensitive detection with a large amount of fingerprint information for the identification of biological materials. In this study, the SERS substrate with silver nanoparticles adsorbed onto glass is a tool that can accurately distinguish bacteria from small amounts without damage of the bacteria. Details on analysis of bacteria based on SERS will be discussed.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-165**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Two-dimensional correlation analysis of formation process of HAMLET

PARK YUJEONG, yeonju Park, subin lee, jieun choi, HEEJIN KIM, Young Mee Jung *

Department of Chemistry, Kangwon National University, Korea

Identification of protein stability, folding / unfolding mechanisms and protein structural changes can provide fundamental knowledge in the study of disease caused by protein denaturation. A representative whey protein, α -lactalbumin undergoes a molten globule state at a certain pH. Under specific conditions, α -lactalbumin and oleic acid form a complex named HAMLET (human α -lactalbumin made lethal to tumor cells). To understand the formation process of HAMLET, it is important to understand the denaturalization process of α -lactalbumin. Therefore, in this study, the structural change of α -lactalbumin with pH change was confirmed by Raman spectroscopy. Changes in Raman spectra were analyzed using principal component analysis (PCA) and two-dimensional correlation spectroscopy (2DCOS). As a result, the mechanism of the denaturalization of α -lactalbumin could be identified at the molecular level.

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Code: **PHYS.P-166**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Computational study on the aromaticity-induced regioselectivity in the synthesis of heterocyclic-functionalized carbazole

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Department of Chemistry, University of Ulsan, Korea

Regioselectivity is of great importance in organic synthesis in order to effectively achieve only a desired material, excluding unnecessary materials. Thus, fundamental understanding the regioselectivity is a long-standing issue in organic synthesis. In this computation study, we study the influence of aromaticity on the regioselectivity of functionalized-carbazole synthesis process via C-acylation-cyclization, through density functional theory (DFT) calculations. In order to unveil the molecular electronic structures, we perform the molecular orbital analysis, the nuclear magnetic resonance simulation, and natural bonding orbital analysis. It was revealed that the stability at the step of formation of iso-carbazole plays an important role in determining the final product. In particular, the aromaticity of heterocyclic rings is inconsistent with the stability of final products. We believe that our study can contribute to the regioselective organic synthesis of carbazole derivatives, which are recently receiving much attention as an ingredient of organic photo-devices, due to their thermally activated delayed fluorescence (TADF) phenomenon.

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Code: **PHYS.P-167**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Control over oligomerization and its molecular motion using protein units

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Abstract Molecular switch, a basic feature of a molecular machine, is an organic compound whose structure can be altered by certain signals. It is one of the research topics that have been recently gaining much attention in nanotechnology, biotechnology (small molecule reference), due to its potential ability to control biological functions such as allosteric regulation. There also have been efforts to produce various molecular machines, with protein being highlighted as an extremely attractive material for designing molecular switch due to its low toxicity inside cells and molecular precision. However, such research efforts have concentrated much on the level of small organic molecules, and there are not many protein-based molecular switches in existence. Furthermore, controlling protein molecular motion still remains as a challenge of protein engineering chemistry. We have created a new protein machine (circular PYP oligomers which can be several doze) which can change the size of the structure upon blue light irradiation in a controllable way. Circular structure of PYP oligomer and its structural change upon irradiation was revealed with STM, TEM and TA,SAXS, TR-WAXS respectively. Here, we have shown clearly the structural change of pyp tetramer in response to light with proper regulation. This research is a step toward producing complex multi-functional protein nano-robots. Also, this would greatly pave way for understanding the molecular functions of a protein and in development of cage molecules and optogenetics tools.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-168**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Monte Carlo Simulation studies in Diffusion-Influenced Reaction for Reaction Rate

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Even though the imperfect trap problems have a large variety of applications in physics, chemistry, and biology, it is not easy to relate the experimental reaction rate to the reaction probability in computer simulations since the relationship between the two is ambiguous yet. By comparing theoretical and simulation results, we try to establish the simple relationship between two parameters in one, two, and three regular dimensions. This can increase greatly the versatility of the lattice-based Monte Carlo simulation methods to be straightforwardly applied to more realistic diffusion-reaction systems.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-169**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Prediction of Chlorosulfolipid (Danicalipin A) Membrane Structure Using Hybrid Molecular Dynamics Simulations

Junyeol Lee, Rakwoo Chang*

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Chlorosulfolipids (CSL) are the major components of flagellar membrane in sea algae. Unlike typical biological lipids with a hydrophilic head group and hydrophobic hydrocarbon tail, CSLs are well known as lipids containing the sulfonate group and chlorines in the head group and hydrocarbon tail group. Among the CSLs, Danicalipin A, Malhamensilipin A, and Mytilipin A are representative lipids. However, it was impossible to isolate Danicalipin A from the alga because of the lack of technology when it was first identified. 40 years later, the research on CSLs have attracted renewed attention by several groups because of their toxicity. It was reported that Malhemensilipin A inhibits bacterial growth and the lysis of mammalian erythrocytes. Mytilipin A is also known as the poison such as yessotoxin that is responsible for human seafood poisoning. Until now, however, there is not enough structural information of CSLs that reveals how the CSLs play biological roles. Thus, we combined coarse-grained (CG) and atomistic molecular dynamics (MD) simulations to obtain some insights into the CSL membrane structures. First, The CG model based on Martini force fields was used to predict the mesoscopic membrane structure of CSLs. We observed that unlike the other CSLs, Danicalipin A forms a stable monolayer membrane structure. Based on these results, we performed atomistic MD simulations of the corresponding atomistic model and obtained a stable CSL membrane structure, in which the CSL lipids adopt a bent structure. In addition, we calculated the membrane thickness, area per lipids, and order parameter to show the membrane integrity. These results provide the significant information to understand the CSL membrane structure.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-170**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Interlayer exciton energy in MX₂ hetero p-n junction

Yongchul Kim, Geunsik Lee*

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

Atomically thin transition metal dichalcogenides MX₂ (M=Mo, W, and X=S, Se) have been studied intensively because of their strong interaction with light, possessing great potential for optoelectronic applications such as photodiodes, photovoltaic cells and light-emitting devices. Recently the vdW p-n heterointerfaces with the type II band alignment have been fabricated successfully with a remarkably fast separation of photoexcited electron and hole carriers, less than 50~100 fs for the hole transfer from MoS₂ to WS₂ layer. However the interlayer exciton binding energy is considered to be significant as its lifetime was measured to be ~1 ns which is still three orders of magnitude shorter than that of bulk silicon (~1 us). Here we calculate the exciton binding energies of MoS₂/WS₂ heterobilayer by using the density functional theory method together with GW and BSE methods. Calculated results are discussed regarding to experimental findings and an approach for weakening the interlayer exciton is suggested towards high performance photovoltaic cells.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-171**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Inverse Charge in Neutral Ag-Au Alloy

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¹*Department of Biomedical Science and Engineering, Sangmyung University, Korea*

Silver-gold (Ag-Au) alloy is one of the most special elemental pairs in nature. Both elements have many properties in common, including their valence electron configuration ($d^{10}s^1$) and lattice constants (Ag: 4.086 Å, Au: 4.072 Å), which results in full miscibility of Ag-Au alloy regardless of its size and composition. On the contrary, the two elements show markedly different electrophilic properties such as electron affinity (Ag: 1.30 eV, Au: 2.31 eV) and electronegativity (Ag: 1.93, Au: 2.54), which allows considerable local polarization of electrostatic charge in Ag-Au alloy. Normally, in the bulk or surface of Ag-Au alloy, it is general that silver atoms have a positive charge and gold atoms have a negative charge due to the difference in their electron affinity and electronegativity. We recently found an inverse case, however, with Ag and Au respectively charged negative and positive, during our quantum mechanical study of the bulk and surface Ag-Au alloy systems. A simple explanation for such a counterintuitive phenomenon is to be presented.

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Code: **PHYS.P-172**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Color change of upconversion emission in NaYF₄:Yb³⁺,Er³⁺ film by phonon relaxation

Lim SooYeong, Chan Ryang Park¹, Hyung Min Kim^{*}

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Upconversion phosphors including rare earth metal atoms emit high energy light under absorb low energy light. It is therefore possible to convert invisible infrared light into visible light. Therefore, the fabricated 2-dimensional patterns of upconversion phosphors can be used in the security or information field. In this study, we tried to prepare upconversion security films which is transparent and emits various colors of light with near IR excitation. With conventional nanoparticle synthesis, it takes a long time to adjust the color and to prepare 2-dimensional patterns. In order to overcome this problem, a monochromatic up-conversion material was fabricated on a thin substrate introduced by pulsed laser deposition (PLD) method. Unlike the conventional method, the emission color of the substrate can be controlled by post-treatment after deposition. Consequently, we produced various color emissions from green to yellow, orange, and red, and the origin of continuous upconversion emission change was elucidated with FT-IR, XPS, and time-resolved photoluminescence method.

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Code: **PHYS.P-173**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Ultrasmall D-glucuronic acid coated Lanthanide (Dy and Ho) oxide Nanoparticles for T₂ MRI Contrast Agent

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Contrast agents are used since the beginning in Magnetic resonance imaging (MRI) to improve the image contrast, as they have great influence in water proton relaxation times T₁ and T₂. Several mechanisms have been proposed to synthesize water soluble T₁, T₂ based MRI contrasting agents. In this study we synthesized ultrasmall Dysprosium oxide and Holmium oxide nanoparticles coated with water soluble and biocompatible D-glucuronic acid. Nanoparticles were characterized by measuring their particle diameter, hydrodynamic diameter, surface coating, r₁ and r₂ values, map images, and in vitro cellular toxicity using different characterization techniques. In this study, the magnetic property and their potential as T₂ MRI contrast agent has been studied.

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Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

MRI contrast Enhancements Using Ultrasmall Gadolinium Oxide Nanoparticles Coated With Dextran

Xu Miao, Gang Ho Lee*

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It was great interest in nanobiology and medicine that nanoparticles with high biocompatibility and stability, low toxicity, diversification of imaging modality, and specificity of targeting to desired organs or cells. In this work, ultrasmall gadolinium oxide (Gd_2O_3) nanoparticles coated with dextran were prepared through one-pot synthesis and their potential to act as a T_1 MRI contrast agent was investigated. The longitudinal (r_1) and transverse (r_2) water proton relaxivities were estimated to be 12.2 and 29.3 $s^{-1}mM^{-1}$ ($r_2/r_1=2.4$) which is larger than those of commercial Gd-chelates. The sample was characterized by HRTEM, FT-IR, TGA, XRD, relaxivity, Map image, Cytotoxicity and in vivo test. The nanoparticles exhibited non-cytotoxicity up to 100 μ M concentration and showed the positive contrast-enhancement on mouse liver and kidneys after the injection of nanocolloid in vivo MRI. Hence, it can be used as a MRI imaging agent.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-175**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dye-coated Gadolinium Oxide Nanoparticles for MRI-FI imaging Agents

Sung June Kim, Gang Ho Lee *

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MRI is important technique in diagnosing diseases and MR imaging agents are also important in order to getting enhanced MR images. We wanted to study synthesizing nanoparticles that has two properties T_1 magnetic resonance images and fluorescent images. So we synthesized dye-coated gadolinium oxide nanoparticles. These dye-coated gadolinium oxide nanoparticles have very good relaxivity for T_1 magnetic resonance imaging and suitable for fluorescent imaging. this study shows high contrast T_1 MR images in vivo, and strong fluorescent images.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-176**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

D-Glucuronic acid coated Bismuth Oxyiodide and Tantalum oxide nanoparticles for CT contrast agent

Adibehalsadat Ghazanfari, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

Molecular imaging is a vital tool for the diagnosis of diseases such as cancers. Among various imaging modalities, x-ray computed tomography (CT) is very useful technique. In this work we reported the synthesis, characterization and application of D-Glucuronic acid coated Bismuth Oxyiodide and Tantalum oxide nanoparticles for CT contrast agent. The characterization result shows that all the particles are monodispersed in size, shape and highly crystalline in nature. The goal of this work is to examine the effect of the surface coating of Bismuth Oxyiodide and Tantalum Oxide nanoparticles. All the synthesized metal oxide nanostructures were characterized by transmission electron microscopy, powder X-ray diffraction and IR spectroscopy. These findings indicate that the nanoparticles reported in this study may be promising CT contrast agents.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-177**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Potential tumor-targeting magnetic resonance imaging: Cyclic RGD-gadolinium oxide nanoparticles

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In this study we investigate tumor targeting T₁ magnetic resonance imaging (MRI) contrast agents. The developed nanovector consists of ultrasmall Gadolinium Oxide (Gd₂O₃) Nanoparticles (GNPs) coated with cRGD. A simple one-pot synthesis of all five cRGD peptide-conjugated ultrasmall GNPs to provide water solubility and to enhance biocompatibility. Peptides play a crucial role in fundamental physiological and biochemical functions of life, It is smaller than most nanoparticles and thus allow for multiple nanoparticle modification and creation of pluripotent nanoparticles. Targeting of nanoparticles in vitro, in cells and in vivo requires nanoparticle surface functionalization. Paramagnetic properties of the cRGD-GNPs and their ability as contrast agents are demonstrated. The sample was characterized by HRTEM, XRD, XPS, FTIR spectroscopy and 1.5 tesla MRI Scanner techniques. These cRGD-GNP samples exhibited longitudinal water proton relaxivities ($r_1 = 10.0 - 18.7 \text{ s}^{-1}\text{mM}^{-1}$ and $r_2/r_1 = 1.4 - 1.7$) higher than those of commercial Gd-chelates. The main purpose of using cRGD as a ligand because it binds with receptor and target specifically within cytoplasm.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-178**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

DFT Simulation of reaction pathways for ammonia addition or subtraction reactions involving N=C or N=N double-bond compounds catalyzed by pincer-type amido hydride Ir complex

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Aforementioned organometallic complex was proposed to catalyze ammonia addition across organic double bonds through both experiments and simulation studies. Here, we report simulation results for the reaction pathways of the ammonia addition across the imine C=N double bond, and the subtraction from hydrazine and aminohydrazine N=N double bond, catalyzed by the present N-H bond activation catalyst. Ammonia subtraction is more favorable for three N-atom containing aminohydrazine than two N-atom containing hydrazine, mainly because the N=N double bond forming reaction step involves only rearrangement of electronic structure with minimal nuclear movements for the former case, while hydrogen-atom migration is invoked for the latter case. In the same manner, the formation of diaminomethane, which is an analog of aminohydrazine, faces essentially no barrier during the reaction pathway.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-179**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

DFT study of organometallic luminophores

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Luminescent organometallic-based luminophores have been extensively studied as promising materials in the field of optoelectronic devices such as organic light-emitting diodes and photovoltaics because of their intriguing optical properties. We have performed density functional theory (DFT) calculations in order to investigate the optimized geometries, the frontier molecular orbitals, and the electronic transitions for organometallic luminophores. All calculations for the compounds were performed at the B3LYP/6-31G(d) level of theory. To include the solvent effect, the conductor-like polarizable continuum model (CPCM) were used. Through comparisons with experimental data, several issues are addressed and discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-180**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dynamic Interactions of Cyclic Peptides with Gram-negative Bacterial Outer Membrane Systems: A Molecular Dynamics Study

Yeonho Song, Hyonseok Hwang*

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Generally, bacteria have the cell wall out of the cell membrane. In the case of Gram-negative bacteria, an outer membrane exists in the outer part of the cell wall. The outer leaflet of the Gram-negative bacterial outer membrane mainly consists of lipopolysaccharide(LPS) and the inner leaflet consists of phosphoethanolamine(PE), phosphoglycerol(PG) and cardiolipin(CL) lipid molecules. In this study, first of all, we examine the thermodynamic and structural properties of Gram-negative outer membranes using all-atom molecular dynamics simulations. Secondly, we assess dynamic interactions of cyclic peptides, $6\times[-D-Arg-L-Arg-[D-Leu-L-Trp]_2-]$, with Gram-negative outer membranes, which will provide insight into the deformation mechanism of the outer membranes and concomitant cell death induced by the cyclic peptides.¹

1.S. Fernandez-Lopez, H. Kim, E. C. Choi, M. Delgado, J. R. Granja, A. Khasanov, K. Kraehenbuehl, G. Long, D. A. Weinberger, K. M. Wilcoxon, and M. R. Ghadiri, Antibacterial agents based on the cyclic D,L- α -peptide architecture. Nature 412, 452 (2001).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-181**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Unusual NO binding to hemoglobin identified by infrared spectroscopy

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Nitrogen monoxide (NO) acts as a physiological messenger regulating local responses of the cardiovascular, immune, and neural systems. It was suggested that a small amount of hemoglobin (Hb) is nitrosylated in the thiol of one β -Cys-93 (S-nitrosylated Hb, HbSNO) and HbSNO is a circulating source of NO that promotes vasodilation in response to reduced O₂ concentration. Since NO can bind much strongly to the ferrous heme, the mechanism for the formation of HbSNO remains unknown. Recently we observed two NO stretching bands of nitrosylated Hb at 1781 cm⁻¹ and 1755 cm⁻¹. When NO bound to the Fe(II) of heme in Hb (HbNO), NO stretching band appears at 1615 cm⁻¹. The new peaks near 1765 cm⁻¹ are not present in myoglobin that does not have cysteine but they appear at a mixture of Fe(II) and S-nitrosothiol (RSNO). When HbSNO is photolyzed, both bands show immediate bleach and recover with the same kinetics of $0.52 \exp(-t/11 \text{ ps}) + 0.48 \exp(-t/430 \text{ ps})$. While the rebinding kinetics is independent of the pump wavelength, the relative magnitude of the bleach depends on the pump wavelength. These two bands may arise from NO bound to β -Cys-93 of Hb: the band at 1755 cm⁻¹ is syn isomer and the band at 1781 cm⁻¹ anti one. We will present the implication of the NO bond structure and rebinding dynamics of NO to the physiological role of Hb as a NO transporter.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-182**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Analysis of Conformational Difference in Mitochondria by UV irradiation in Skin-originated Cells and Tissues Using STED Nanoscopy

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Division of Chemistry, Seoul National University, Korea

Since the sub-structure of mitochondria may reflect mitochondrial activity in various cellular environment, we applied super-resolution STED nanoscopy to examine UV-induced morphological dispersion of mitochondria both in sub-cultured human primary skin fibroblasts and mouse skin tissues. In the sub-cultured fibroblasts, confocal microscopy provides overall morphology of mitochondrial outer membrane by TOM20 (translocase subunit on the mitochondrial outer membrane) within diffraction limit. Using super-resolution STED nanoscopy, however, we were able to resolve different distributions of TOM20 clusters induced by UV irradiation in the cells and tissues.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-183**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Adsorption structure of ethanol on Ge(100)

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Chemical reaction of ethanol with semiconductor surface has been investigated using density functional theory (DFT) calculations. Calculated results show that, at room temperature, O-H dissociative adsorption is kinetically more favorable than C-O dissociative adsorption, although the final product of C-O dissociative adsorption produces thermodynamically more stable product. Thus the surface adsorption of ethanol on Ge(100) is dominated by kinetic control rather than thermodynamic control at room temperature. The activation barriers for the reaction pathways well calculated with climbing nudged elastic band method. Simulated images from the OH-dissociative structures are consistent with experimental STM images at room temperature. From the results of our DFT calculations, we conclude that the adsorption structure of ethanol on Ge(100) at room temperature has a H-Ge-Ge-OC₂H₅ geometry as a result of O-H -dissociative adsorption on a single dimer.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-184**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Multi Theragnostic Agent Using Ultrasmall Gadolinium Oxides Nanoparticles Coated With Poly(Acrylic Acid)-Rhodamine

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Theragnostic agents are compounds that able for both diagnosis and therapy of diseases, which catching a lot of interest because they provide more advantages than a single-modal agent. In this work, ultrasmall gadolinium oxides nanoparticles which were coated with poly(acrylic acid)-rhodamine showed not only excellent magnetic resonance imaging properties but also great fluorescent and pH-reponsive ability, due to the presence of rhodamine moiety. Furthermore, these Gd₂O₃ NPs are also applied for gadolinium neutron capture therapy (GdNCT) on human glioblastoma U87MG cells and showed good result *in vitro*.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-185**

Area: Physical Chemistry

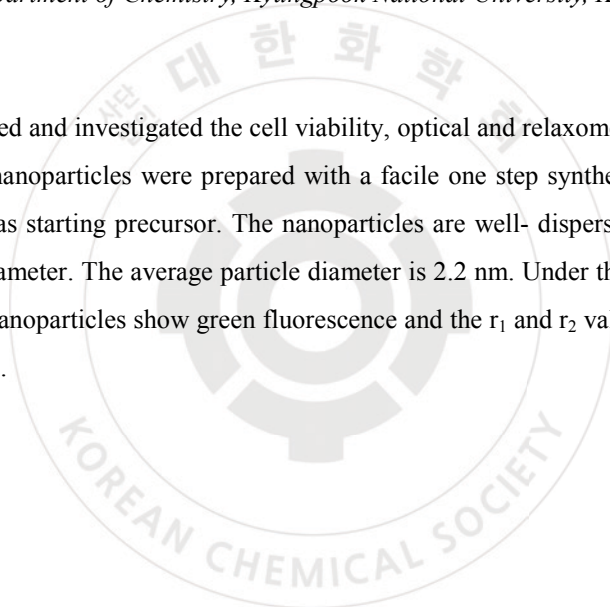
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Characterization of Fluorecent carbon nanoparticles

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In this study, we prepared and investigated the cell viability, optical and relaxometric properties of carbon nanoparticles. Carbon nanoparticles were prepared with a facile one step synthesis method in a solution by using carbohydrate as starting precursor. The nanoparticles are well- dispersed in distilled water and ultrasmall in particle diameter. The average particle diameter is 2.2 nm. Under the irradiation of UV light at 365 nm, the carbon nanoparticles show green fluorescence and the r_1 and r_2 values were estimated to be 0.036 and $0.068\text{s}^{-1}\text{mM}^{-1}$.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-186**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of Hybrid Nanostructures Comprising Perovskite (Ba₅Nb₄O₁₅)-MoS₂ Ultrathin Nanosheets on CdS Nanorods: Toward Enhanced Solar-Driven H₂ Production

EunHwa Kim, Amaranatha reddy, Sangyeob Hong, Hanbit Park, Rory Ma, PRAVEEN KUMAR DHARANI, TaeKyu Kim *

Department of Chemistry, Pusan National University, Korea

Solar-driven semiconductor-catalyzed photocatalytic water splitting is an significant and eco-friendly chemical technique for the production of clean hydrogen fuel. However, a cost-effective, efficient photocatalyst with perfect photon-to-hydrogen molecule conversion remains elusive. Novel, noble-metal-free hybrid nanostructures comprising perovskite (Ba₅Nb₄O₁₅)-MoS₂ ultrathin nanosheets on CdS nanorods, with efficient photo-charge separation and migration capability for efficient solar-driven hydrogen production are designed. The nano-hybrid structures display a high hydrogen production rate of 147 mmol·g⁻¹·h⁻¹ in the presence of lactic acid as a sacrificial electron donor under simulated solar irradiation; this value is much higher than those of the CdS/MoS₂ (124 mmol·g⁻¹·h⁻¹) and CdS/Ba₅Nb₄O₁₅ (18 mmol·g⁻¹·h⁻¹) nanostructures and that of the expensive CdS/Pt benchmark catalyst (34.98 mmol·g⁻¹·h⁻¹). The apparent quantum yield at 425 nm reaches to 28.2% in 5 h. Furthermore, the rate of solar-driven hydrogen evolution in the presence of the ultrathin perovskite Ba₅Nb₄O₁₅/MoS₂ nanohybrid on the CdS nanorods is much faster than that of several noble-metal-free co-catalyst-modified CdS nanostructures reported earlier. UV-Vis absorption, photoluminescence, photocurrent, and impedance analyses of CdS@Ba₅Nb₄O₁₅/MoS₂ reveal that the high photocatalytic hydrogen evolution rate may due to the comparatively higher solar light-harvesting capacity and efficient charge separation and migration, which reduces the recombination rate. We anticipate that the presented design strategy for the development of noble metal-free catalysts combining perovskite and semiconductor nanostructures stimulate the development of diverse non-precious robust solar light-harvesting noble-metal-free materials for water splitting to satisfy the growing global energy demand.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-187**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Comparative Study on the Binding Characteristics of p53-mimicking Peptides to HDM2

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Tumor suppressor protein p53 cannot be activated and do its function upon binding with HDM2 protein. Inhibition of the p53/HDM2 interaction is thus significant for suppressing the growth of tumor cell. Recently, the stapled p53 peptide and the cyclized helix-loop-helix peptide (cHLH) mimicking the α -helix part of p53 protein have been designed and found to exhibit high binding affinity with HDM2. Here, we report the structural and thermodynamic characteristics for the binding complex of the cHLH/HDM2, stapled p53/HDM2, and unstapled p53/HDM2 complexes. We performed molecular dynamics simulations to investigate the structural properties of the three complexes. The binding free energy calculations based on the integral equation theory was then executed to quantify the binding affinity for the three protein complexes and to understand the factors responsible for the binding affinity. Additionally, we compared the binding properties between the cHLH/HDM2, stapled p53/HDM2, and unstapled p53/HDM2 in order to provide more suitable inhibitors of the p53/HDM2 complex.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-188**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The DFT Calculation for DMMP-Thiourea Derivatives Complexes

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Dimethyl methylphosphonate (DMMP) is widely used as a test chemical for mimicking numerous nerve agents. Binder molecules to sense DMMP efficiently has been developed in many laboratories. To aid the development, the binding strengths of numerous thiourea derivatives with DMMP are calculated with the density functional theory (DFT). More than 20 starting geometries per target/binder complexes were obtained using molecular dynamics calculation and optimized with the B3LYP-D3/6-31+G* level of theory. The hydrogen bonding and CH/ π interaction are two dominant factors for the binding process. We investigated for thirty-one thiourea derivatives, some of which are in Figure. We found that the binding strengths of benzyl or 3,5-bis-trifluoromethylphenyl derivatives of thiourea, such as TU4, TU8, TU24, and TU28 in Figure, are higher than other derivatives. These results are consistent with experiments employing quartz crystal microbalance.

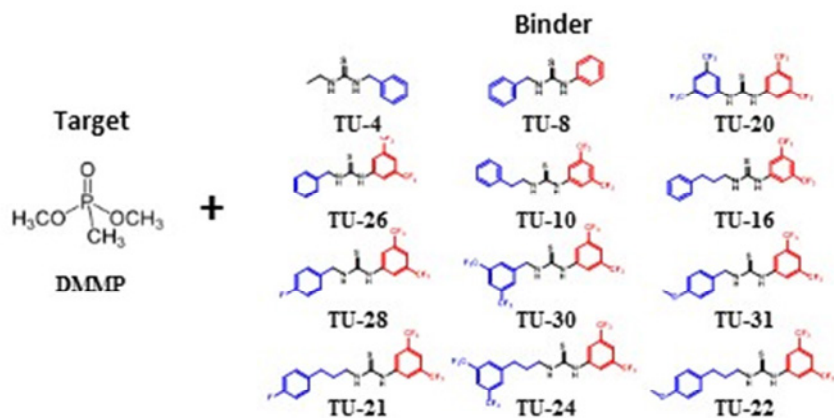


Figure. Structures of DMMP as the target molecules and thiourea derivatives as binder molecules

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-189**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Atomic-level Investigations on the Interaction between Amyloid- β and Tau with Explicit Water

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Senile plaques of amyloid- β ($A\beta$) and neurofibrillary tangles (NFTs) of Tau are pathological hallmarks of Alzheimer's disease (AD). However, the early stage of $A\beta$ interacting with Tau to form insoluble complexes in intracellular space has still been limited. Herein, we have presented unguided, explicit-water, all-atom molecular dynamics (MD) simulations and solvation thermodynamic analysis results on the dimerization process between Tau43 and $A\beta$ 42 in aqueous environments. Two-stage approaching-accommodation mechanism driven by protein internal force from individual diffusive regime at large separations to form compact dimer structures is observed in the Tau43- $A\beta$ 42 dimerization pathway. Remarkably, the mid-to-C-terminal region of $A\beta$ 42 (especially the C-terminal region 39VVIA42) well binds to Tau43 in dimeric complexes through hydrophobic interactions, which is in good agreement with experimental results and contribute to the understanding of tau pathogenesis induced by $A\beta$ 42 not $A\beta$ 40. Our results thus provide the driving force and structural origin for the early $A\beta$ -Tau aggregation on the atomic level in aqueous environments.

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Code: **PHYS.P-190**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Comparison of Monte Carlo and Brownian Dynamic Simulations for Diffusion-Influenced Reactions

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In this work, we compare Monte Carlo simulation methods with those of Brownian dynamics. Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. Their essential idea is using randomness to solve problems that might be deterministic in principle. They are often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other approaches. Monte Carlo methods are mainly used in three distinct problem classes optimization, numerical integration, and generating draws from a probability distribution. Brownian dynamics simulation is to mimic the Brownian motion of molecules in liquid or on surface. Following the dynamics including the random force instead of Newtonian motion, we can enhance the efficiency of the simulations. Here, focusing on the efficiency of both simulation methods, we study advantages and disadvantages of both simulation methods for diffusion-influenced reaction.

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Code: **PHYS.P-191**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Ancillary ligand effect on Inter-Ligand Energy Transfer in the Heteroleptic Iridium Complex: Comprehensive investigations of its fast dynamics and mechanism

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Department of Advanced Materials Chemistry, Korea University, Korea

A series of heteroleptic Ir complexes which contain two kinds of ligand (two dfppy ligands and an ancillary ligand) were prepared to obtain evidence of the ILET process that can be observed in the presence of energetically different ligands in metal complexes. We introduced two types of ancillary ligands: 1) non-luminescent ancillary ligands, namely tetrakis(pyrazolyl)borate (bor) and picolinate (pic), which were employed for the preparation of Ir(dfppy)₂(bor) and Ir(dfppy)₂(pic), respectively, and 2) luminescent ancillary ligands, namely 1,10-phenanthroline (phen), bipyridine (bpy), and 2,3-dipyridylpyrazine (dpp), which were employed for the preparation of Ir(dfppy)₂(phen), Ir(dfppy)₂(bpy), and Ir(dfppy)₂(dpp), respectively. Based on the study for temperature dependency, the solvent rigidity is very important factor for ILET. The excited states of dfppy are higher than those of phen, bpy, and dpp; thus, ILET occurs from dfppy to the other ligands lying in lower energy states. The ILET dynamics can be determined directly using fs-TA spectroscopy. The ILET properties were affected by several important factors, such as the energy differences between the main and ancillary ligands, the temperature, and the rigidity of the environment.

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Code: **PHYS.P-192**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Reversal of Proton Affinity with Collective Hydrogen-Bonding of Water and Alcohol Clusters

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The photoinduced proton transfer of a series of strong photoacids, N-methyl-n-hydroxyquinolinium ions (NMnHQ⁺) with an acidic hydroxyl group at 3 (NM3HQ⁺), 5 (NM5HQ⁺), 6 (NM6HQ⁺), 7 (NM7HQ⁺) and 8 positions (NM8HQ⁺) to water molecules was systematically studied in acetonitrile, an aprotic medium. We measured excited-state lifetimes of the prototropic species of NMnHQ⁺ using picosecond-resolved fluorescence spectroscopy and analyzed their proton transfer kinetics to reveal the size of water clusters as bases. The results show that the critical sizes of the water clusters are: three for NM7HQ⁺, two for NM3HQ⁺ and NM6HQ⁺, and one for NM5HQ⁺ and NM8HQ⁺. From the Förster analysis modified from its original version [1], the acid dissociation constants in the excited states (pK_a^*) of the photoacids were evaluated and found to correlate with the sizes of the water clusters as bases; the sizes of the water clusters decrease as a photoacid becomes more acidic, i.e., with a lower pK_a^* value. From the comparison with our previous results reporting the sizes of alcohol clusters as Brønsted bases in the acid-base reactions of the same photoacids [2-4], it is revealed that water is less reactive in the acid-base reactions than alcohol when hydrogen-bond network is limited to form small clusters. References: [1] Tolbert, L. M.; Solntsev, K. M. *Acc. Chem. Res.* 2002, 35, 19-27. [2] Park, S. Y.; Lee, Y. M.; Kwac, K.; Jung, Y.; Kwon, O.-H. *Chem. Eur. J.* 2016, 22, 4340-4344. [3] Lee, Y. M.; Park, S. Y.; Kim, H.; Kim, T. G.; Kwon, O.-H. *Methods Appl. Fluoresc.* 2016, 4, 024004. [4] Park, S. Y.; Kim, T. G.; Ajitha, M. J.; Kwac, K.; Lee, Y. M.; Kim, H.; Jung, Y.; Kwon, O.-H. *Phys. Chem. Chem. Phys.* 2016, 18, 24880-24889.

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Code: **PHYS.P-193**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Study of steric effect on excimer formation in planar Pt(II) complexes

Yang-Jin Cho, So-Yoen Kim, DAE WON CHO, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In order to understand the steric influence on the excimer formation in square planar metal complexes, three different Pt(II) complexes were prepared by modifying the substituents in the main ligand: Pt(II)(dfppy)(acac) (Pt-1, where dfppy is difluorophenylpyridine, acac is acetylacetonate); the bulky triphenyl silyl (Ph₃Si-) group was substituted at the pyridine moiety (Pt-2) and at the phenyl moiety (Pt-3) of the main ligand of Pt-1. The Pt-complexes showed sky-blue emission at ~460 nm. In addition, Pt-1 and Pt-3 showed excimer emission at ~600 nm in the concentrated solution and the solid sample. The emission lifetimes and intensities for monomeric Pt-1 and Pt-3 showed strong concentration dependence. Indeed, the lifetime of the monomer was reduced in highly concentrated solutions due to excimer formation. The intrinsic emission lifetimes were determined as 364 ns (Pt-1) and 300 ns (Pt-3) by Stern-Volmer analysis, considering the self-quenched lifetime of monomer emission. Pt-2 did not show any excimer emission in the concentrated solution or solid sample. The crystal structures of Pt-1 and Pt-3 were analysed by X-ray crystallographic measurements. The results revealed that the LUMO moiety was closely overlapped with that of another Pt-complex. In this study, based on the influence of steric hindrance of the bulky Ph₃Si group, we concluded that the LUMO-LUMO interaction between the pyridine moieties of the main ligand is the main factor responsible for excimer formation.

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Code: **PHYS.P-194**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fluorescence Protein for Long-term Live-cell Super-resolution Imaging of Various Cellular Structures

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

UnaG is a fluorescent protein discovered from Japanese Eel, whose fluorescence arise only when the protein binds to bilirubin (BR), a nonfluorescent metabolite. We investigated UnaG's photoswitchable nature caused by repetitive binding and unbinding of BR. Mainly the photooxidation of BR induces the off-switching of UnaG fluorescence. When the damaged BR is exchanged to fresh one, the protein recovers the fluorescence capability. Since more than 50% of UnaG molecules can survive after >300 switching cycles, UnaG should be an attractive candidate for a fluorescent probe for single-molecule localization based super-resolution imaging, especially for the long-term live-cell imaging. We imaged various UnaG labeled subcellular structures with sub-diffraction limit resolution in live Cos7 cells. As a result, we can increase the number of super-resolution snapshots more than 10 times with UnaG than conventional fluorescent probes (except lipophilic dyes that have limited applications).References[1] A. Kumagai, R. Ando, H. Miyatake, P. Greimel, T. Kobayashi, Y. Hirabayashi, T. Shimogori and A. Miyawaki, Cell, 153, 1602 (2013).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-195**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dependence of Proton Transfer Dynamics on the Configuration of Diols as Effective Brønsted Bases

Ye-Jin Kim, Oh-Hoon Kwon^{*}

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

As viscous hydroxylic organic compounds, diols are of interest for their functional molecular conformation, which is based on inter- and intramolecular hydrogen (H)-bonds. By utilizing steady-state electronic vibrational spectroscopy, time-resolved fluorescence spectroscopy, and computational analyses, we report the association of the hydroxyl groups of diols via intra- or intermolecular H-bonds to enhance their basicity. Whereas the formation of an intermolecularly H-bonded dimer is requisite for diols with weak intramolecular H-bond to extract a proton from a model strong photoacid, a well-configured single diol molecule having strong H-bond is revealed to serve as an effective Brønsted base with increased basicity. This was evidenced by quantum chemical calculations, where the observed proton-transfer rate for the well-configured H-bonded complex is correlated well with the intramolecular H-bond length of a diol molecule. This observation highlights the collective role of H-bonding in acid-base reactions, and provides mechanistic backgrounds to understand the reactivity of polyols in acid-catalyzed dehydration for the synthesis of cyclic ethers at the molecular level.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-196**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Live-cell Imaging of Alkyne Groups by Raman Microscopy Vibrational Probes with Alkyne Groups for Imaging of Cellular DNA

Hee-Chang Kim, Giseong Lee, Hogyu Han, Sang-Hee Shim*

Department of Chemistry, Korea University, Korea

The alkyne group ($C\equiv C$) has a characteristic vibrational mode in the range of $\sim 2100\text{ cm}^{-1}$, where is considered as the 'silent region' for cell imaging applications, allowing high molecular contrast for chemical imaging of biological samples. Here we introduce an efficient hyperspectral method for Raman imaging by utilizing the advantage of alkyne. Attaching additional small functional groups to the alkyne causes resolvable shift in the vibrational frequency, while the frequency remains in the silent region. In order to precisely tune the vibrational frequency, we synthesized various 5-ethynyl-2'-deoxyuridine (EdU) based alkyne-(small functional groups) combinations by using trimethylsilyl (TMS), conjugated diynes ($-C\equiv C-C\equiv C-$), etc. These products showed clearly shifted vibrational frequencies, as well as successful cellular uptake, resulting a high contrast hyperspectral cellular imaging.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-197**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Thermal stability and free-energy landscape of DNA hairpin structure d(ATCCAT-GTTA-TAGGAT) using molecular dynamics simulation

Hyun Jung Yoon, Sangwook Wu *

Department of Physics, Pukyong National University, Korea

DNA hairpin plays a critical role in the regulation of gene expression and DNA recombination. We studied the stability of the DNA hairpin structure, d(ATCCAT-GTTA-TAGGAT) (PDB id:1AC7) using molecular dynamics (MD) simulation. Despite the non-canonical Watson-Crick base pair (G:A) in the tetraloop (GTTA), we found that the conformation of the DNA hairpin is remarkably stable. In this study, we attempted to understand the origin of the stability of DNA hairpin with 2-dimensional free energy landscape in the conformational space composed of dihedral angles along DNA backbone chain.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-198**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Enhanced Photocatalytic Activity of Au-doped Au@ZnO Core-Shell Flower-like Nanocomposites

Ravindranadh Koutavarapu, hyeon jin Jung, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, India

The abundant importance to photocatalytic activity is the effective charge separation and interfacial charge transfer in the semiconductors. In this work, we introduce a simple and low cost three-step hydrothermal and pulsed laser ablation method for the synthesis of the flower-like ZnO, Au@ZnO core-shell and Au@ZnO core-shell nanocomposites doped with various concentrations (5, 10 and 15 wt.%) of Au nanoparticles, to enrich the catalytic performance of ZnO under UV irradiation. Compared to the other prepared samples, Au@ZnO core-shell nanocomposites with 5 wt.% of Au dopant exhibit a better enhancement in the photocatalytic activity. The structural and spectroscopic measurements of the prepared materials were studied by X-ray diffraction (XRD) and UV-vis investigations. From the XRD pattern of the prepared samples, two crystalline phases of hexagonal ZnO and face-centered cubic structure of Au are observed. Further, the morphology of the as synthesized nanocomposite was studied by field-emission scanning electron microscopy and high-resolution transmission electron microscope imaging and the elemental analysis was explored by using energy dispersive X-ray spectroscopy, respectively.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-199**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dependence of Hydration Dynamics on the size of a Water Pool in a Reverse Micellar System Probed by a Superphotoacid

Jae-Heon Park, hak-won Nho, Oh-Hoon Kwon*

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

Reverse micellar (RM) system is a representative molecular biomimetic system. The characteristics of RM systems varies with the size of the RMs, mainly the size of nano-size water pools. The water pool can be further divided into two different regions: boundary water and free water. In the boundary water region, the water molecules have strong dipole-ion interaction with the surfactant head groups, so that the boundary water motion is more restricted than that of free water motion. On the other hand, the mobility of water molecules in the free water region becomes similar with that of bulk water. Here, we investigated the hydration characteristics in the water pool of Aerosol-OT (sodium bis[2-ethylhexyl] sulfosuccinate) RMs by measuring the time-resolved fluorescence of cationic superphotoacid, N-methyl-7-hydroxyquinolinium ion (NM7HQ⁺) in the water pool. NM7HQ⁺ is a strong photoacid with a much lower pK_a value than in the ground state when excited by light which triggers the excited-state deprotonation of the cationic NM7HQ⁺ (C) giving birth to a product, keto form (K). The two prototropic species have different formal charges, which affect residence sites and diffusive motions in the confined environment of the RMs. The excited-state dynamics of NM7HQ⁺ was analyzed by measuring picosecond resolved emission spectra (PRES). The spectral deconvolution of the PRES into the spectra of the two prototropic species allowed for the differentiation of the time dependent spectral shift from the excited-state population dynamics. As a result, we successfully resolved the hydration dynamics in the water pool and correlated it with proton-transfer dynamics. In addition, we calculated the kinetic isotopic effect for excited-state proton transfer by comparing the lifetimes obtained on PRES in H₂O and D₂O pools. Also, the time-resolved fluorescence anisotropy measurements revealed the rotational/translational diffusion dynamics of the two prototropic species in RM.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-200**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Modeling of Super-Resolution Imaging of Single Molecule in Plasmonic Gap

Gyu Jin Yeon, Gyouil Jeong, Yun-gi Kim, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

Using finite-difference time-domain electrostatics method, physical validity of super-resolution imaging of single molecules in plasmonic gap with surface-enhanced Raman scattering (SER) has been investigated. The calculation reveals that displacement of center of point-spread function (PSF) in image plane is linearly proportional to the molecular displacement of a single molecule (modeled as a point-dipole emitter) across a plasmonic gap-axis. The observed behavior disagrees with the conventional belief in SERS that the eigen-mode-like plasmon mode would result in negligible sensitivity on the positions of a single molecule in the gap. The anomalous behavior can be interpreted as retardation effect of bonding quadrupole mode and consequent asymmetry in the phase of far-field emission.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-201**

Area: Physical Chemistry

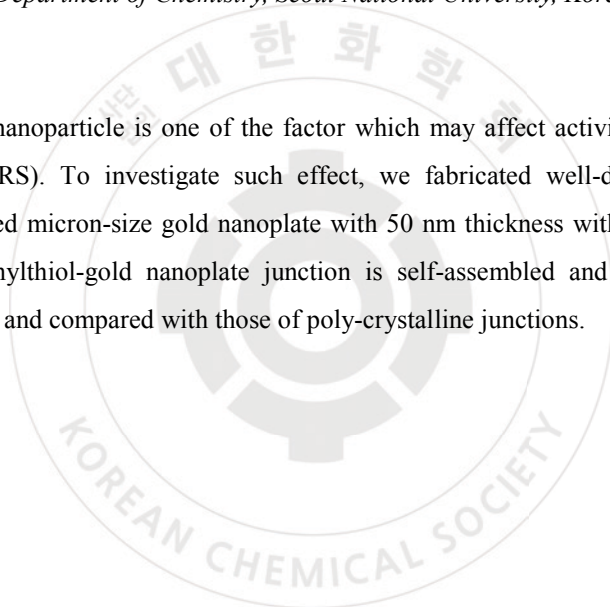
Type: Poster Presentation, Time: FRI 13:00~14:30

Generation of SERS hotspots with single-crystalline junction

Seung Yeon Lee, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

Crystal-facet of metal nanoparticle is one of the factor which may affect activities of surface-enhanced Raman Scattering (SERS). To investigate such effect, we fabricated well-defined single-crystalline junction. We synthesized micron-size gold nanoplate with 50 nm thickness with atomically flat surface. Silver nanocube-biphenylthiol-gold nanoplate junction is self-assembled and SERS activities of the junctions are measured, and compared with those of poly-crystalline junctions.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-202**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Real-time single-molecule SERS monitoring for tautomerization reaction of hypoxanthine

Kang Sup Lee, Zee Hwan Kim^{*}

Department of Chemistry, Seoul National University, Korea

We monitored tautomerization reaction of single or a few molecules of hypoxanthine (HX) on metallic surfaces (Ag nanoparticle/HX/Au thin film junction) using single-molecule SERS ($\lambda_{\text{ex}} = 632.8 \text{ nm}$). The SERS spectra of two HX tautomers show distinct spectral features at $\nu_1 \approx 720 \text{ cm}^{-1}$, (ketonic form, acidic) and $\nu_2 \approx 740 \text{ cm}^{-1}$ (enolic form, basic). We observe discrete transitions between ν_1 -only and ν_2 -only peaks, which may reflect the tautomerization reaction events of single or very few HX molecules. The pH influence on the SERS trajectories is examined to validate our hypothesis.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-203**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Protein network analysis of a conformational change for c-Src tyrosine kinase

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Department of Physics, Pukyong National University, Korea

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

Tyrosine kinase c-Src plays a critical role in numerous cellular signaling pathways. Activation of c-Src involves a change from its inactive to the active state depending on the phosphorylation state of two major phosphorylation sites, Tyr416 and Tyr527. In this study, we investigated the inactive to active conformational change of c-Src using molecular dynamics simulation. Based on the MD simulation, we proposed a dynamical scenario for the activation process of c-Src. A detailed analysis of dynamical protein network reveals that Lys321 has the highest scores in centrality measures (degree and betweenness) during the activation process. Based on network analysis, we suggest that Lys321 plays a key role in the c-Src activation process.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-204**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Vibrational mode competition in three-color stimulated Raman scattering (SRS) spectroscopy

doyeon Kim, Sang-Hee Shim*

Department of Chemistry, Korea University, Korea

Stimulated Raman Scattering (SRS) can obtain much enhanced scattering cross section (about seven orders of magnitude) than normal Raman scattering. Conventional SRS uses two-waves, pump and Stokes light, to detect molecular vibrational mode. The previous studies tuned the pump and Stokes wavelength to make vibrational coherence, and obtained vibrational information of molecules. To investigate the interaction between two different SRS processes, we implement a three color SRS experiment which enables to simultaneously induce two different vibrational coherence of two SRS process in the same molecule: the pump and one Stokes light is resonant to a vibrational mode; the pump and another Stokes light is resonant to a different vibrational mode. We observed competitive behavior of two SRS processes, in which one SRS process can suppress another SRS process, for the first time. The depletion phenomenon is induced only when both the two different SRS modes are resonant to Raman transitions. Our experimental results also indicate that SRS depletion is caused by confined amount of pump photons. We obtained up to 62% efficiency of depletion of the ring breathing mode of benzene by using the CH stretching mode for depletion. With these experimental data, we expect this new switching-off concept for SRS has a potential to be practically used in various area, like the study for molecular energy redistribution, etc.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-205**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

SERS Imaging of line hotspots of silver nanowire dimer

Sang-Min Park, Kang Sup Lee, Gyu Jin Yeon, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

We observed an oscillating pattern in the wide-field surface-enhanced Raman scattering (SERS) images of biphenyl-4-thiol molecules sandwiched between two near-contact silver nanowires (NW-dimer): a focused laser illumination ($\lambda_{\text{ex}} = 632.8$ or 532 nm) at the terminus of NW launches surface plasmon polariton (SPP) propagation to form delocalized SERS patterns along NW-axis. We hypothesize that such unusual SERS patterns arise from interference of higher-order SPP modes of NW-dimers, producing oscillating intensity distributions. The hypothesis is validated by the simulation based on local field distributions at NW-gap and the SERS radiation pattern arising from a point-dipole emitter.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-206**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Designing Open-pore 3D CdS Mesoporous Networks on Metal-Organic-Framework-derived Co Nanocrystal-Embedded Few-layered Carbon@Co₉S₈ Double-Shelled Nanocages

Amaranatha reddy, Hanbit Park, MADHUSUDANA GOPANNAGARI, EunHwa Kim, TaeKyu Kim*

Department of Chemistry, Pusan National University, Korea

Designing porous nanostructures with unprecedented functions and an effective ability to harvest the maximum energy region of the solar spectrum and suppress the charge-carrier recombination rate is offering promising potential for sustainable energy production. Although several functional porous nanostructures have been developed, high-efficiency materials must still be developed. Herein, we report a new, highly active, noble-metal-free, and redox-mediator-free Z scheme photocatalyst, CdS/Co-C@Co₉S₈, for hydrogen production through water splitting under solar irradiation. The designed photocatalytic system contains open 3D CdS mesopores as a light absorber for wider solar light harvesting. Metal-organic-framework-derived cobalt nanocrystal-embedded few-layered carbon@Co₉S₈ double-shelled nanocages were used as a co-semiconductor to hamper the photo charge-carrier recombination by accelerating the photogenerated electrons and holes from the other semiconductor. The optimized catalyst shows a hydrogen evolution rate of 26.69 mmol•g⁻¹•h⁻¹ under simulated solar irradiation, which is 46 times higher than that of as-synthesized CdS mesoporous nanostructures. The spectacular photocatalytic activity of CdS/Co@C-Co₉S₈ reflects the favorable suppression of the charge-carrier recombination rate, as determined by photoluminescence, photocurrent, and impedance analyses. We believe that the findings reported here may inspire the design of novel noble-metal-free porous nanohybrids for sustainable green hydrogen production.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-207**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Frequency-Domain Proof of Existence of Atomic-Scale SERS Hot-Spots

Hyun-Hang Shin, Gyu Jin Yeon, Sang-Min Park, Kang Sup Lee, Ja-Jung Koo, Seung Yeon Lee, Zee Hwan Kim^{*}

Department of Chemistry, Seoul National University, Korea

The existence of sub-nm plasmonic hot-spots and their relevance in spectroscopy and microscopy applications remain still elusive, despite a few recent theoretical and experimental evidences supporting this possibility. Here we present new spectroscopic evidence that angstrom-sized electromagnetic hot-spots exist on the surfaces of plasmon-excited nanostructures. The surface-enhanced Raman scattering (SERS) spectra of 4, 4'-biphenyl dithiols placed in metallic junctions show simultaneously blinking Stokes and anti-Stokes spectra, some of which exhibit only one prominent vibrational peak. The activated vibrational modes are found to vary widely between junction-sites. Such site-specific, single-peak spectra could be consistently modeled by single-molecule SERS process induced by hot-spots with sizes no larger than 2.5 Å in radii, located at specific molecular sites. Furthermore, the model, which assumes the stochastic creation of hot-spots on locally flat metallic surfaces, faithfully reproduces the intensity distributions and occurrence statistics of the blinking vibrational peaks, further supporting that the sources of hot-spots are located at the metallic surfaces. The result not only provides another compelling evidence for the existence of angstrom-sized hot-spots, but it also opens up possibilities for regio-specific photo-excitation of a single molecule, and for real-space visualization of molecular vibrational modes.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-208**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Conformationally Resolved Spectroscopy of Jet-cooled methacetin

Cheol Joo Moon, Yeonguk Seong, Jihyun Park, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

The excitation spectra of jet-cooled methacetin (MA) have been measured by using combination of mass-selected resonant two-photon ionization and ultraviolet-ultraviolet hole-burning (UV-UV HB) spectroscopy in the gas phase. Four different UV-UV HB spectra originated from two conformers of MA (syn- and anti-MA) with its fundamental and hot transition of each have been obtained. The IR-dip spectroscopy has conclusively confirmed the coexistence of the two rotamers with an aid of theoretical calculations. The vibronic band assignments in the low frequency region having internal rotation of methyl group of methyl-capped peptide, attributed from the 1e rotational level, are presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-209**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Conformationally Resolved Structures of Indole-3-acetic Acid in the Gas Phase

Yeon Guk Seong, Cheol Joo Moon, Jihyun Park, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Indole-3-acetic acid (IAA) is the most common plant hormone that plays an essential role in the regulation of plant growth and fruit development. The special role in nature has led us to investigate the intrinsic properties of IAA in the gas phase. The current research provides the complete conformational assignments of indole-3-acetic acid (IAA), which has three conformers in the gas phase. In this work, we have measured the electronic spectra of IAA by employing a resonant two-photon ionization (R2PI) and UV-UV hole-burning (UV-UV HB) technique in the free jet conditions. We have identified three lowest-energy conformers of IAA (Inp-Py-Out, Oop-Py, and Oop-Ph) with an aid of a combination of R2PI, UV-UV HB, IR-dip spectroscopy, and density functional theory calculations. Based on the results presented here, we have re-visited the conformational assignments of IAA conformers, which were previously assigned by the rotational spectroscopic study of IAA.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-210**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

TiO₂@Au Nanoparticles Produced by Pulse Laser Irradiation for Photocatalytic Activity

Seung Heon Lee, Hyeon Jin Jung, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

TiO₂@Au nanoparticles have various applications such as photocatalysis, solar energy conversion, chemical and biological sensing. Among various particle fabrication methods, pulsed laser irradiation in liquid (PLIL) is currently attracting great interest due to its simplicity and versatility. In this study, TiO₂@Au nanoparticles via PLIL were synthesized and their morphological and optical properties were characterized by X-ray diffraction, field emission - scanning electronic microscope, energy dispersive spectrometer, high resolution - transmission electron microscope and UV-Vis spectroscopy. Additionally, other TiO₂@M (M=Pt, Pd, Ag) nanoparticles will be synthesized and applied for the photodegradation of organic dye compounds under UV and visible light conditions.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-211**

Area: Physical Chemistry

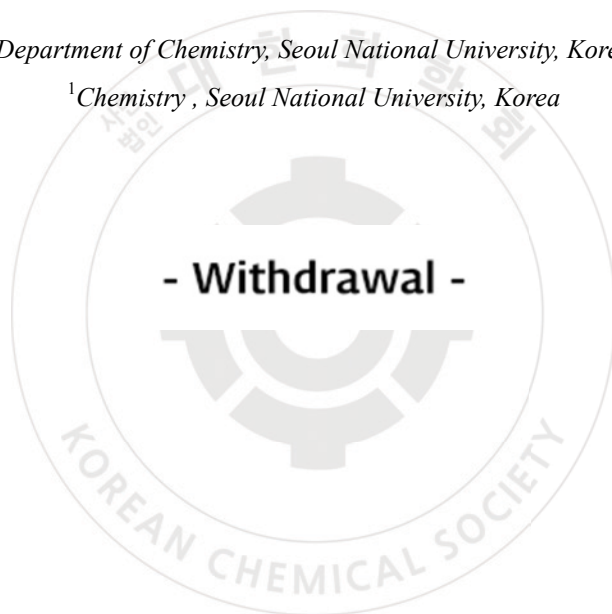
Type: Poster Presentation, Time: FRI 13:00~14:30

[Withdrawal] Ultrafast plasmon-phonon relaxation dynamics of individual metal nanoparticle

Boogeon Choi, JiWon Park¹, Zee Hwan Kim^{*}

Department of Chemistry, Seoul National University, Korea

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120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-212**

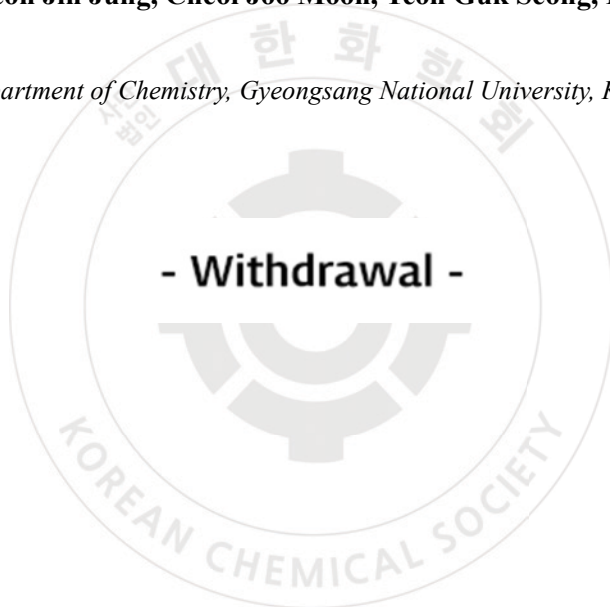
Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

[Withdrawal] Low Temperature Photoluminescence Studies of ZnO and Zn@ZnO Core-shell Nanoparticles Produced by Pulsed Laser Ablation in Liquid

Jihyun Park, Hyeon Jin Jung, Cheol Joo Moon, Yeon Guk Seong, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-213**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Enhanced Degradation of Methylene Blue Using Pd-TiO₂ Bimetallic Nanofibers

Dayeon Lee, Hyeon Jin Jung, Myung Hwa Kim¹, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

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

Recently TiO₂ has been gaining huge attention as photocatalyst due to its economic efficiency and good photocatalytic activity. To increase photocatalytic activity of TiO₂ we ablate laser to the solution of TiO₂ anatase nanofibers, prepared by an electrospinning method, and palladium chloride (PdCl₂). This process has been prepared via pulsed laser ablation in liquid (PLAL) which is a simple one-step preparation method and easy way to make nano particles. After the PLAL process, the end of TiO₂ nanofiber transfer to rutile phase and palladium-TiO₂ bimetallic materials were fabricated. We varied the percentage of palladium chloride in the mixture (5%, 10%, 15%, and 20%) to find out the most efficient photocatalytic activity. The Pd-TiO₂ nanofibers showed an enhanced photocatalytic activity for decomposing methylene blue, compared with pure anatase TiO₂ nanofibers without palladium. More detailed experimental Pd-TiO₂ nanofibers analysis of the photocatalytic activities will be characterized by using transmission electron microscope, scanning electron microscope, and UV-vis spectrophotometer and presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-214**

Area: Physical Chemistry

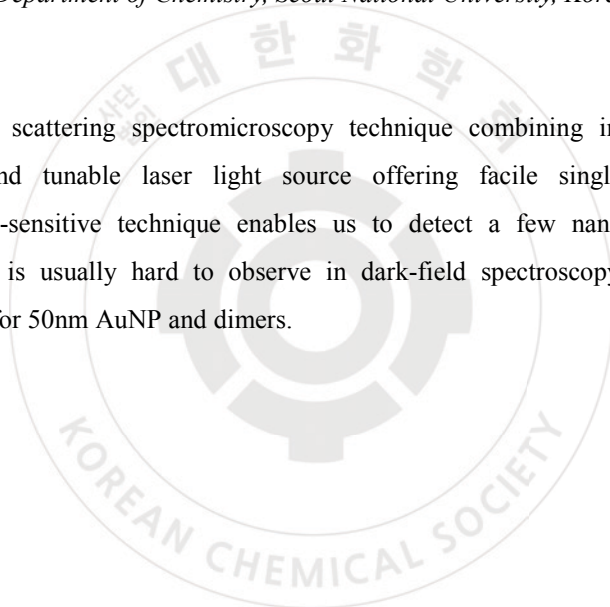
Type: Poster Presentation, Time: FRI 13:00~14:30

Interferometric scattering spectroscopy and microscopy

Hankyul Lee, Sungi Kim, Boogeon Choi, JiWon Park, Jwa-Min Nam^{*}, Zee Hwan Kim^{*}

Department of Chemistry, Seoul National University, Korea

We developed a new scattering spectromicroscopy technique combining interferometric scattering microscopy(iSCAT) and tunable laser light source offering facile single-particle tracking and characterization. Phase-sensitive technique enables us to detect a few nanometer scale plasmonic resonance shift which is usually hard to observe in dark-field spectroscopy. An example of such capability is presented for 50nm AuNP and dimers.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-215**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Pulsed Laser Ablation Synthesis of Graphitic and Nitrogen-doped Graphitic Layers Produced from Solvents on Nickel Nanoparticles

Hyeon Jin Jung, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Graphite-encapsulated Ni nanoparticles (NPs) have been fabricated at room temperature and atmospheric pressure by a one-pot synthesis by pulsed laser ablation to Ni plate submerged in a solvent, which acted as the carbon source. The formation of graphite- and N-doped graphite-encapsulated Ni nanoparticles (Ni@C and Ni@N-C NPs) was simply achieved by pulsed laser ablation in the solvent, of which hexane and acetonitrile were used for the carbon and nitrogen-doped carbon source, respectively. Meanwhile, Ni and Ni@NiO NPs were fabricated by pulsed laser ablation in methanol and deionized water, respectively. The characterizations of these Ni NPs were analyzed by X-ray diffraction measurements, X-ray photoelectron spectroscopy, field emission scanning electron microscopy, high-resolution transmission electron microscopy, fast Fourier transform analysis, selected area electron diffraction, and Fourier transform Raman spectroscopy. From the above analysis, plausible mechanisms for the surface modified Ni NPs are presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-216**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Physicochemical characteristics of a liposomal system incorporated with dual anti-cancer drugs

Hasoo Seong^{*}, Jae Hyun Nam

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

As a delivery system for combination chemotherapy, nano-sized liposomes containing two kinds of drugs with different physicochemical properties such as erlotinib (ERL) and doxorubicin (DOX) in a single liposome vesicle have been studied. In this study, preparation methods and physicochemical properties of a dual drug delivery system based on non-pegylated liposome formulation were investigated to optimize the system. ERL-encapsulated liposomes were prepared using the lipid film-hydration method. By ultrasonication using a probe sonicator, the liposome diameter was reduced to less than 200 nm. The sonication was highly effective for the reduction of liposome diameter when it was performed after the film-hydration and before DOX encapsulation. DOX was efficiently loaded into the ERL-encapsulated liposomes using ammonium sulfate (AS)-gradient method. Equilibration of a mixture of DOX solution and ERL-encapsulated liposomes was effective for enhancement of EE of DOX. The dual drug-encapsulated liposomes with 140 nm of liposome diameter had more than 90% and 30% EE's of DOX and ERL, respectively. TEM revealed that the dual drug encapsulated liposomes were spherical and had crystalline complexes formed between protonated DOX cations and sulfate anions inside the liposomes as analyzed by HR-TEM and selected area electron diffraction pattern. The dual drug encapsulated liposomes showed a time-differential release of ERL and DOX, implying the releases of the drugs in a proper sequence for synergistic effects. These results on physicochemical properties of the dual drug delivery system suggest a basis for optimization of preparation process and translational researches of the system showing synergistic effects of the drugs.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-217**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Optical Second-Harmonic Generation Spectroscopy of 2-Dimensional ReSe₂

Gwanghyun Ahn, Sunmin Ryu*

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

Various semiconducting 2-dimensional crystals including transition metal dichalcogenides (TMDs) have recently been studied for nonlinear optical properties and applications. In particular, non-centrosymmetric TMDs exhibited strong optical second-harmonic generation (SHG) with their 2nd-order nonlinear susceptibility surpassing that of conventional nonlinear crystals. In this work, we explored SHG phenomenon in thin 2-dimensional rhenium diselenide (ReSe₂) crystals that are known to have inversion symmetry. 800 nm output of a Ti:Sapphire oscillator with 140 fs pulse width was used as a excitation fundamental beam. Thin ReSe₂ crystals were directly grown on SiO₂/Si substrates via chemical vapor deposition. Despite the centrosymmetry associated with the space group (C_i^1) of ReSe₂, strong SHG signals at 400 nm were detected for various thickness between 4 and 10 nm. The SHG signals exhibited quadratic dependence on the intensity of the fundamental beam confirming its 2-photon nature. Polarization-resolved measurements showed distinctive two-fold symmetry. The apparent anomaly of SHG by the centrosymmetric crystal will be discussed considering possible structural distortion, photoinduced effects and multipole contribution.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-218**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Time Evolution of Photoexcited Carriers in 1D/2D nanomaterials

Jaehun Park

Pohang Accelerator Laboratory, Korea

In this paper, the interaction between terahertz light and 1D/2D nanomaterials in nonequilibrium as well as in equilibrium state will be discussed. Si_{1-x}Ge_x nanowires (NWs) were synthesized via a Vapor-Liquid-Solid (VLS) procedure. The optically excited carrier dynamics of Si_{1-x}Ge_x NWs is measured as a function of Ge content using optical pump-THz probe spectroscopy. The measured $-\Delta T/T_0$ signals of Si_{1-x}Ge_x NWs were converted into conductivity in the THz region. Intra- and inter-valley transition times and trapping times of electrons and holes of Si_{1-x}Ge_x NWs will be discussed as a function of Ge content. Chalcogenide based compound, especially Sb₂Te₃ and related compounds, are suitable candidates for rewritable optical storage media and phase change random access memory. We will show the relationship between structural phase transition of {Sb(3)Te(9)}_n thin film from amorphous into crystalline states and the transition of optical properties in THz range using THz-TDS(Terahertz Time Domain Spectroscopy) and OPTP(Optical Pump Terahertz Probe).

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-219**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A portable gas chromatograph for in-situ monitoring of air pollutants

Juyeon Bang, Dong Wook You, KWANG WOO JUNG*

Department of Chemistry, Wonkwang University, Korea

Current study describes a small and light-weight gas chromatograph (GC) system (30×20×15 cm³, 5 kg) for real-time and quantitative determinations of gas mixtures in air sample. The system is integrated with a low thermal mass (LTM) column module, electronic pneumatic (or pressure) controller (EPC), and a miniature photoionization detector. Ambient air is employed as a carrier gas, and a diaphragm pump is used to provide the pressurized carrier gas. We evaluate the reliability of developed equipment by analyzing quantitative and qualitative of gas sample. Performance of the portable GC is compared with the commercial equipment Agilent GC using the same experimental method.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-220**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Orientation-Sensitive Imaging of Anisotropic Particle with New Interferometric Scattering Microscopy-type Method

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Department of Chemistry, Korea University, Korea

Single molecule detection techniques have allowed one to observe biological systems. It is difficult to observe nanoscopic phenomena optically because of diffraction limit of optical detection. To overcome this limit, various super-resolution microscopy, such as fluorescence microscopy, have been developed. Although there are numerous advantages of fluorescence microscopy techniques, they usually suffer saturation of signal, photobleaching and photoblinking of fluorophores. These problems disrupt stable and long-term tracking of targets of interest. Here, we developed new experimental scheme based on interferometric scattering microscopy (iSCAT), which collects the interference between the scattering field from target and the reference field from interface of chamber. We constructed orientation sensitive optical system with linear polarized light and dual camera system. With signal difference between two images of which the linear polarized light is perpendicular to each other, orientational information of nanorod were delivered and also, we observed Brownian rotational motion of a single anisotropic gold nanorod.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-221**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Characterization of Electrical Properties in TFTs with ALD Grown 4MP Doped ZnO

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We proposed and fabricated zinc oxide thin-film transistors (TFTs) employing 4-mercaptophenol (4MP) doped ZnO by atomic layer deposition (ALD) that results in highly stable and high performance. The 4MP concentration in ZnO films were varied from 1.7% to 5.6% by controlling Zn:4MP pulses. The n-type carrier concentrations in ZnO thin films were controlled from $1.017 \times 10^{20}/\text{cm}^3$ to $2.903 \times 10^{14}/\text{cm}^3$ with appropriate amount of 4MP doping. The 4.8% 4MP doped ZnO TFT revealed good device mobility performance of $8.4 \text{ cm}^2/\text{Vs}$ and the on/off current ratio of 10^6 . Such 4MP doped ZnO TFTs exhibited relatively good stability ($\Delta V_{\text{TH}} : 0.4 \text{ V}$) under positive bias-temperature stress while the TFTs with only ZnO showed a $4.3 \Delta V_{\text{TH}}$ shift, respectively.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-222**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Buckingham and Lennard-Jones Potentials for Molten Alkali Halides: Conversion of Born-Mayer-Huggins potential to computationally efficient alternatives

Rushie Mae Cedeno^{*}, Kyung-koo Lee^{*}

Department of Chemistry, Kunsan National University, Korea

Computer simulation that employs the interatomic potential molecular dynamics (IPMD) with Born-Mayer-Huggins (BMH) potential has been the most important technique in studying the properties of molten alkali halides. To further reduce the computational cost for these systems, new sets of Buckingham and Lennard-Jones parameters have been developed through BMH potential conversion using nonlinear curve fitting procedure that uses a Levenberg-Marquardt algorithm to find the local minimum. New systematic fitting schemes are presented that accounts all the like and unlike ion-ion interactions in molten lithium and potassium chloride salts. Also, the Lorentz-Berthelot combination rule, which is conventionally used among these interactions, is considered. The obtained parameters were evaluated by a weighted statistical comparison against the calculated force of BMH potential. Analysis of the fitting results has shown that the parameters can be optimized with a fitting range starting near at the ionic equilibrium distances of LiCl and KCl. Investigation of the simulation results has shown that these optimized weighted parameters of Buckingham can be robust in predicting the density, enthalpy and diffusion coefficients of the molten salts with minimum mean unsigned error (MUE) against the results using BMH potential. On the other hand, the obtained Lennard-Jones parameters may not be as robust as Buckingham parameters but this is due to the intrinsic limitation of the fitting procedure with BMH potential. This work explores the possibility of obtaining computationally efficient alternative parameters that can be readily available for IPMD simulations of molten LiCl and KCl systems.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-223**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Stochastic Photon Emission from Non-Blinking Upconversion Nanoparticles

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Because of their well-known optical properties, upconversion nanoparticles (UCNPs) are regarded as some of the most promising nanomaterials for bioimaging, biosensors, and solar cells. The non-blinking nature of their upconversion emissions has been a particularly beneficial advantage for live-cell imaging. However, the origin of this unique property has never been seriously investigated. We report, for the first time, the observation of stochastic photon emission (SPEM) in core/shell UCNPs (NaYF₄:Yb³⁺,Er³⁺/NaYF₄) on the microsecond and nanosecond time scales, even under continuous irradiation at 980 nm. This SPEM was attributed to slow “upconversion cycles.” We consider that the conventionally reported, non-blinking nature of UCNP emissions can be attributed to the averaging of SPEMs from multiple Er³⁺ ions and the low temporal resolution of previous observation. The off-time distribution, which possesses kinetics information for the upconversion pathways, was well fitted to a single exponential indicating involvement of a single rate-determining step. The distinct behaviors of the green and red emissions confirm their different photophysical pathways.

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Code: **PHYS.P-224**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dye-conjugated Upconversion Nanoparticles for pH-sensing

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Korea*

Intracellular pH-sensing has great importance to understand the cellular activities and early detection of diseases. Therefore, the development of optical pH-sensor that is capable of being employed in the cell, is an urgent demand in medical research and diagnostics. Herein, the dye-conjugated upconversion nanoparticles (UCNPs) based on resonance energy transfer have been presented as a pH-sensing system. By analyzing the ratiometric variation of luminescence emission from the pH-dependent fluorescein dye and pH-insensitive NaYF₄: Tm³⁺/Yb³⁺ UCNPs, we measure the pH of the system. The designed upconversion nanoparticles are suitable for a biological application, as they are known to have high photostability, low cytotoxicity, low photobleaching and lack of autofluorescence in biological material.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-225**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Non-poisson decay has an affect on correlation between expression levels of independent genes

Jaehyuk Won, Jaeyoung Sung*

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We studied analysis of the environment-induced correlation between the expression levels of dual reporter genes A(CFp) and B(mCherry). Our reaction network consider that mRNA and protein degrade with constant decay rate γ_m , γ_p . But, their degradation pathways are complex in reality. We bring in the reaction network composed of vibrant reaction process with the product decay process is multi-step form that each step has constant decay rate γ . We can get the correlation of gene A and gene B when the number of steps N are different.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-226**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Computer Simulation Study of Interaction between Carbon Dots (CD) and Lithium Ions

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Department of Chemistry, Kwangwoon University, Korea

Lithium hexafluorophosphate (LiPF₆) used as a Li⁺ donor in Lithium ion batteries suffers from serious stability problems.¹⁻³ Hence, there have been much interest in replacing it with more stable materials. Recently, researchers have found carbon dots (CD), nano-meter sized graphene oxide molecules, can be the candidate for their high stability and high Li⁺ capacity. In this study we have built up CD models with various numbers of functional groups such as -OH and -COOH and investigated their binding affinity with the Li⁺ ions using molecular dynamics simulations. We have found the carboxyl group is mainly responsible for the strong affinity with Li⁺ ions. We have also calculated the binding free energy of a Li⁺ ion on both CD and PF₆⁻ using metadynamics simulation methods. [1] I. Geoffroy et. al. J. Pow. Sour. 2002, 11, 192-198.[2] C. Zhao et. al. J. Mater. Chem. A 2013, 00, 1-3.[3] J. Zhang et. al. J. Pow. Sour. 2013, 241, 619-626.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-227**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Hydration dynamics of methyladenines, biomarkers of DNA methylating agents

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We have investigated the hydration properties of lithium complexes of methyladenines (3-methyladenine; 3MA, 7-methyladenine; 7MA, 9-methyladenine; 9MA) using a quadrupole ion trap (QIT) mass spectrometer. Methyladenines complexed with a lithium cation were introduced into the vacuum system using electrospray ionization (ESI) and were isolated using MS/MS to react with water molecules within the quadrupole ion trap (QIT). The reaction time changed from 0 to 5 seconds, and the mass spectra after the reaction were recorded as a function of the reaction time. The decay curve of each methyladenine was obtained by measuring the fraction of ion intensity of $[M+Li]^+$ (156m/z) over the total intensity of $[M+Li]^+$ and $[M+Li+H_2O]^+$ (174m/z). The decay curves of lithium complexes of 3MA, 7MA, and 9MA showed distinct values in the decay time constants and the non-reacted fraction determined by the asymptote of hydration decay curve. We will discuss the differences in hydration dynamics of different methyladenine complexes with a lithium cation based on the different hydration decay time constants and fractions of non-reacted species.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-228**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and characterization of ReO₃ doped MoO₃ nanorods

Hyerim Oh, Yukyung SHIN, Myung Hwa Kim*

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

By Chemical Vapor Deposition process using ReO₃ and MoO₃ powder as precursors, we synthesized Rhenium trioxide (ReO₃) doped Molybdenum trioxide (MoO₃) nanorods. The morphology and ratio of grown MoO₃/ReO₃ nanorods can be controlled depending on the ratio of precursor. The morphology and the crystal structure of MoO₃/ReO₃ nanorods were characterized with field emission scanning electron microscope (FE-SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD), Raman spectroscopy and transmission electron microscopy (TEM). The results confirmed that the MoO₃ nanorods were doped with ReO₃ so that it is expected that ReO₃ doped MoO₃ nanorods show the higher electrical conductivity than pristine MoO₃ nanorods.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-229**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of mixed rhodium and cobalt oxide nanofibers by electrospinning process

SOYEON KIM, HAYEON KIM, Myung Hwa Kim*

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

One-dimensional nanofiber of mixed metal oxide, rhodium oxide (Rh_2O_3), cobalt oxide (Co_3O_4), and Cobalt rhodium oxide (Co_2RhO_4) were successfully synthesized by electrospinning process. The crystal structure and morphology of the samples were characterized with field emission scanning electron microscope (FE-SEM), energy dispersive spectroscopy (EDS), transmission electron microscopy (TEM), X-ray diffraction (XRD), and Raman spectra. Results show that the electrospun nanofibers consisting of rhodium and cobalt oxide are formed with the shape of the hollow tube so that it is expected that composite nanofibers could be extended to apply for high efficient electrocatalysts.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **PHYS.P-230**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Ultrafast exchange dynamics of electrolyte in Lithium ion battery

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CMSD-IBS/Department of Chemistry, Korea University, Korea

Electrolyte in lithium ion battery is mixture of lithium salt and carbonate solvents. Lithium ion is the charge carrier, carbonates form stable solvation sheath of Li^+ . Here two-dimensional infrared spectroscopy is applied to study dynamics of electrolyte in lithium ion battery. In LiPF_6 diethylcarbonate(DEC) solution, 2DIR spectra show increasing cross-peaks which means ultrafast exchange dynamics. The exchange time, which are calculated with 2DIR spectra and two state model, are on picosecond timescale. 2DIR spectra of DEC and propylene carbonate(PC) mixed solvent system, cross-peaks are observed as ever at same timescale.

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Code: **PHYS.P-231**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Photochemical Etching of InP Quantum Dots

Hwajun Jeong, Seungtaek Rim, Seung Koo Shin*

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Quantum dots (QDs) prepared by colloidal synthesis usually show a monodisperse but wide size distribution that results in a rather broad emission spectrum. To reduce the emission band width and to tune the emission color, we carried out the photochemical etching of InP QDs. InP QDs were synthesized by a one-pot process and the photochemical etching of as-synthesized InP QDs was performed in chloroform by using a high power 532 nm laser. Photochemical etching processes were monitored by absorption and emission spectroscopy. After photoirradiation, the band-edge wavelength was shifted to blue, indicating the reduction in quantum size. The rate of etching varied with additives. After reducing the size by photochemical etching, resulting InP QDs were overcoated with a layer of ZnS shell, and their optical properties were characterized. The photochemical etching of compound semiconductor QDs is a useful tool to overcome the batch-to-batch variation in colloidal growth processes.

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Code: **PHYS.P-232**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Solvent Polarity Effect on Exciplex Conformation on Linked Electron D-A Molecules

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In photo-induced electron transfer (PET) strong interaction of excited acceptor-donor pair produces radical ion pair (RIP) or excited state charge-transfer complexes, which is called exciplex. Generation of RIP or exciplex is dependent on solvent polarity. Exciplex emission band of pyrene-(CH₂)₁₂-O-(CH₂)₂-N,N-dimethylaniline was observed to decrease in intensity and be red-shifted with solvent polarity. This type of behavior is explained by solvent polarity effect in electronic structure of exciplex. We assume that polar solvent transform exciplex conformation from planar structure into twisted like intramolecular charge transfer structure. In order to search for transformation of exciplex we synthesized pyrene-COO-(CH₂)₁₁-O-(CH₂)₂-N,N-dimethylaniline and we observed that difference between two molecules in degree of charge separation in a same polar solvent. Quantum mechanical calculation provided corresponding molecular structures. Our assumption of the solvent polarity effect on the exciplex conformation was tested by synthesizing pyrene-(CH₂)₁₂-O-(CH₂)₂-julolidine which was twisted conformation was prohibited.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **PHYS.P-233**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Through-Space Ultrafast Photoinduced Electron Transfer Dynamics of a C₇₀-Encapsulated Bisporphyrin Covalent Organic Polyhedron in a Low-Dielectric Medium

Jaehong Park

Department of Molecular Engineering, Kyoto University, Japan

Ultrafast photoinduced electron transfer (PIET) dynamics of a C₇₀-encapsulated bisporphyrin covalent organic polyhedron hybrid (C₇₀@COP-5) is studied in a nonpolar toluene medium with fluorescence and transient absorption spectroscopies. This structurally rigid donor (D)–acceptor (A) molecular hybrid offers a new platform featuring conformationally predetermined cofacial D–A orientation with a fixed edge-to-edge separation, R_{EE} (2.8 Å), without the aid of covalent bonds. Sub-picosecond PIET ($\tau_{ET} \leq 0.4$ ps) and very slow charge recombination ($\tau_{CR} \approx 600$ ps) dynamics are observed. The origin of these dynamics is discussed in terms of enhanced D–A coupling ($V = 675$ cm⁻¹) and extremely small reorganization energy ($\lambda \approx 0.18$ eV), induced by the intrinsic structural rigidity of the C₇₀@COP-5 complex.

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Code: **PHYS.P-234**

Area: Physical Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Three-Photon-Induced Fluorescence Microscopy using Tryptophan

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People have been interested to observe the inside of intact cells or tissues for a long time. However, it is challenging to get the high spatial-resolution deep tissue image due to the strong scattering of most biological samples in conventional microscopy. Multi-photon fluorescence microscopy is a useful tool for whole cell and in-vivo tissue imaging, because it overcome this problem with near-infrared light region that provides less scattering, less phototoxicity and deep penetration depth. Moreover, intrinsic small excitation volume generation of multi-photon excitation process enables optical sectioning for 3D image reconstruction. In this poster, we report the recent progress in three-photon-induced fluorescence (3PIF) microscopy. Ultimately, we would like to report the 3D imaging by the 3PIF from tryptophan (Trp), a potential intrinsic fluorescent dye in a biological system. Trp has absorption and emission peaks at 280 nm and 350 nm, respectively. These UV absorption and emission have hindered people from using Trp as fluorescent dye. We expect to avoid this problem by three-photon absorption process. For showing our microscopy 3PIF PSF, we used 100 nm fluorescent bead that has UV absorption and visible emission peak at 260 nm and 450 nm, respectively. It shows that our microscopy has xxx nm lateral resolution and xxx nm axial resolution at 1000 nm excitation wavelength through 60x objective lens (water immersion, NA 1.2). Also to show the 3D imaging ability, we imaged glass beads in Trp monomer solution .

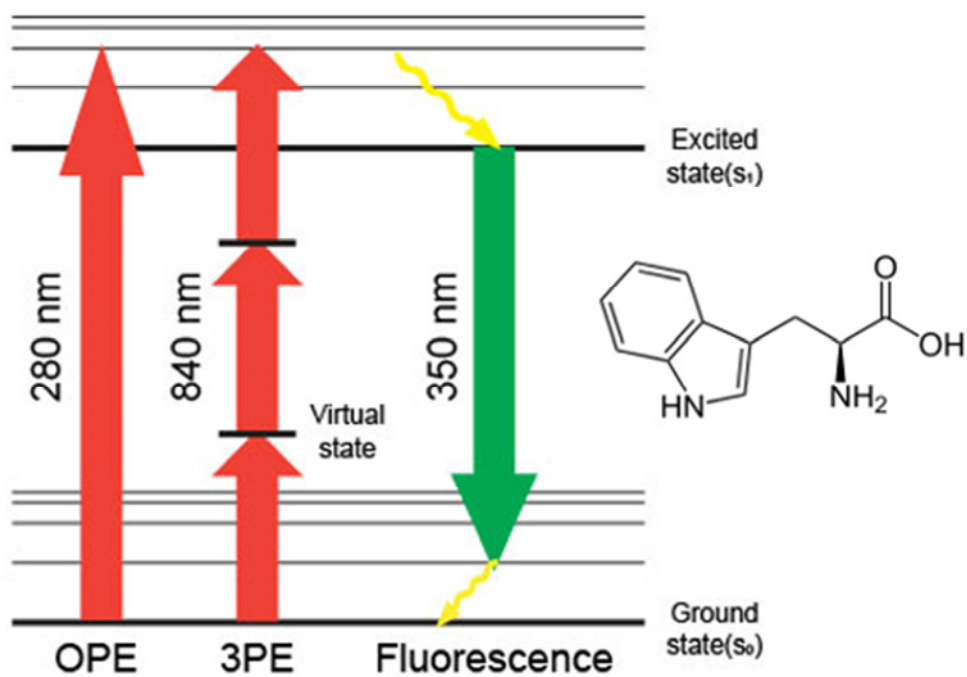


Figure 1. Jablonski diagram of one photon excitation, three photon excitation and fluorescence of Tryptophan⁺



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Code: **ANAL.P-152**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A colorimetric probe to determine NO₂⁻ using label free gold nanocrystals

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A simple and sensitive colorimetric method for the determination of NO₂⁻ ions in aqueous samples was developed using gold nanocrystals (AuNCs). The NO₂⁻ ion is selectively etched AuNCs and changing the particle shape. This etching resulted in a dramatic color change from vivid blue to light red. Using this methodology, the concentration of NO₂⁻ ions in environmental, biological and sitological samples could be quantitatively detected by the naked eye or by using UV-Vis spectrometry. Also, we found that the selectivity and sensitivity of the detection was noticeably improved at the 20mM of NaCl concentration, at which a more obvious color change was observed. The absorption ratios (A₅₅₀/A₆₅₀) of the modified AuNCs solution exhibited a linear correlation with NO₂⁻ ion concentrations within the linear range of 0.0~10 ppm, and the limits of detection in tap water, pond water and waste water were 38.45 nM and 0.46 μM, respectively. This cost-effective sensing system allows for the rapid and facile determination of NO₂⁻ ions in aqueous samples.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL.P-153

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Analysis of Correlation between Structure of Linear Surfactants and Acute Eye Irritation Scores

Sujin Cho, Tian Tian, Seog Woo Rhee *

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In this work, we determined the eye irritation scores of surfactants with linear alkyl chains by HET-CAM assay using hen's eggs and investigated the correlation between the structure of surfactants and eye irritation scores. Surfactants with a cationic (ammonium salt), neutral, anionic (sulfate) head groups and a linear alkyl chain with 8 to 16 carbons as the tail group were selected. The properties of surfactant forming micelles in aqueous solution were measured by an electrical conductivity method and an absorbance measurement method. The eye irritation scores of surfactants at various concentrations were measured by the HET-CAM assay using hen's eggs as an alternative animal test. Based on the experimental results, we found a significant correlation between the structural properties of the surfactant and the critical micelle concentration, and the acute irritation score of the surfactant. The results of this study will be used to develop cell-based devices using microfluidic chips that can replace the HET-CAM assay.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL.P-154**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Assessment of Phototoxicity Inhibition of Flavone-based Materials

Sung Eun Lee, Tian Tian, Seog Woo Rhee*

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In this work, we investigated the phototoxicity inhibition process of flavone-based materials using the 3T3 NRU assay, an in vivo acute phototoxicity evaluation method. Amiodarone HCl and chlorpromazine HCl were used as phototoxic materials, and chrysin and apigenin were used as photoinhibition inhibitors. The phototoxicity index, PIF value and MPE value, were calculated based on the cell viability measured as a function of concentration. When cells were treated with solutions containing both chlorpromazine and flavone-based materials, both chrysin and apigenin reduced the phototoxicity of chlorpromazine by UVA. In addition, we will discuss the cytotoxic and phototoxic mechanisms of each material and the phototoxicity inhibition process of flavone-based materials.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-155

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Sequential colorimetric detection technology of iron and mercury ions by etching and aggregation of gold nanorods

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¹*Green City Technology Institute, Korea Institute of Science and Technology, Korea*

A simple and sensitive colorimetric assay method for the sequential determination of iron ions and mercury in aqueous samples was developed using label free gold nanorods. Iron ions etched gold nanorods, and mercury ions bond these gold nanorods together. This sequential react results in a dramatic color change from red to blue and finally back to red. Therefore, the concentration of iron ions and mercury ions in environmental samples can be quantitatively detected by the naked eye or by UV-Vis spectrometry when using the AuNRs sensor. The sensitivity of the detection is significantly improved by modulating the solution to pH 7, leading to a more rapid color change in the optimized AuNRs system. The absorption ratios (A_{640}/A_{740}) of the modified AuNRs solution exhibited a linear correlation with the iron ion concentrations. The absorption ratios (A_{550}/A_{640}) of the modified AuNRs solution exhibited a linear correlation with the mercury ion concentrations, with a limit of detection of 25.2 nM. This cost-effective detection system allows for the rapid and facile determination of the concentration of iron ions and mercury ions in aqueous samples.

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Code: ANAL.P-156

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Morphological elucidation of porous PCL(Polycaprolactone) microsphere using various analytical methods

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The surface and internal morphology of biodegradable PCL(Polycaprolactone) microsphere was investigated in order to understand how can the porosity be distributed. The PCL microsphere were manufactured for medical use. The size distribution was measured by electrical sensing zone type particle size analyzer. And the surface porosity was observed using SEM. For the inner pore observation, first we confirmed that there were inner pores in the microsphere by OM. But PCL's low melting point of around 60°C and a glass transition temperature of about -60°C made it difficult to observe the cross-sectional image of the inner pore. It means that the conventional technique such as Microtome and cryo-CP methods were not available for PCL microsphere cross-section image and inner pore evaluation. We applied some ideas for solving this problem. Total porosity of PCL microsphere was measured using Mercury Porosimeter. Then we recalled the Mercury intruded samples and made cross-sectional cuts easily in the LN2 environment thanks to the occupied Mercury volume. The inner and under surface pore was observed using EDS mapping Mercury image. The micro-CT technique was not applicable in this study because of the mismatching spatial resolution.

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Code: ANAL.P-157

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Effect of Adsorbate Molecules on Chemical Interface Damping in Single Gold Bipyramids with Sharp Tips

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Single metallic nanoparticles are gaining much attention as an attractive biomolecular sensor. Especially, gold bipyramids (AuBPs) are expected to be a promising material for biosensors to have high detection sensitivity due to its sharper tips compared with spherical gold nanoparticle or rod-shape gold nanoparticle. They have higher sensitivity to refractive index of attached target molecules than spherical gold nanoparticles and gold nanorods. However, the conventional localized surface plasmon resonance (LSPR) sensing mechanism is affected by both the change of dielectric medium constant and the chemical adsorption onto the nanoparticle surface. Herein, we performed single particle spectroscopic study to characterize the effect of the medium dielectric constant and chemical binding of various thiol molecules on the LSPR linewidth in single AuBPs. More specifically, we demonstrate how chemical binding of various adsorbate molecules affects the LSPR linewidth of the longitudinal surface plasmon of single AuBPs. We found that the LSPR linewidth of single AuBPs remains almost constant when varying the refractive index of surrounding medium. However, thiol binding resulted in the redshift and broadening of LSPR spectrum of single AuBPs. Therefore, the results suggest that chemical interface damping of single AuBPs can be used to develop a LSPR biosensor that is only sensitively to the adsorption of biomolecules without interference from the dielectric constant of the surrounding medium.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL.P-158**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Decontamination of sulfur mustard in sand, concrete, and asphalt matrices

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The persistence of sulfur mustard is still a major challenge for decontamination, as it remains in the environment after longer intervals of time. Decontamination involves multiple mass transport mechanisms, such as diffusion and chemical interactions among a contaminant, a decontaminant, and material interfaces. The complex series of interacting processes can contribute to post-decontamination hazards, such as vapor emission and contact transfer to humans and the environment. The present work is concerned with the decontamination of sulfur mustard on sand, concrete, and asphalt. This array of matrices was chosen to represent complex surfaces commonly observed in an urban environment that would be expected to be easily targeted by terrorists or rogue organizations. The results show that the whole amount of the mustard agent was not decontaminated, and 2 ~ 3 % of the preliminary quantity remained after the decontamination process, which was emitted as vapor over time. Not only vapors of the residual agent but also its byproducts, including sulfoxide and sulfone compounds, were gradually emitted from the decontaminated surface over time. For such byproducts, the hypochlorite ion (OCl^-), an active ingredient in the decontaminant used, reacts with sulfur mustard by oxidation to sulfoxide and/or sulfone and by dehydrochlorination to form such compounds as divinyl sulfone, which are reported to be relatively nontoxic.

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Code: **ANAL.P-159**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Surface-Enhanced Raman Scattering of Gold Nanourchins with Sharp and Short Branches

MINJUNG SEO, JI WON HA*

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Raman spectroscopy is a useful technique to observe vibrational, rotational, and other low-frequency modes in a system. Raman spectroscopy is complementary with IR and can be used when IR is forbidden. But, spontaneous Raman scattering is typically very weak compared with Rayleigh scattering because Raman intensity is almost 0.001% of the source intensity. Therefore, it is important to develop methods to enhance the signals. SERS (Surface Enhanced-Raman Scattering) is one of the methods that can enhance the signals up to 10^{11} . It is the basic principle of SERS that enhances Raman scattering by molecules adsorbed on rough metal surfaces or nanostructures. Various conditions are required for SERS. In the present study, we tried to optimize SERS with gold nanourchins (AuNUs) having sharp tips and rough surface. We tried SERS effect with R6G, p-aminothiophenol as probe molecules, 100-nm AuNUs. Raman spectra were measured with confocal homemade-Raman spectroscopy, and a 785-nm diode laser was used as a radiation source. LSPR peak of 100-nm AuNUs is close to 785-nm laser for resonance effect.

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Venue: Kimdaejung Convention Center, Gwangju

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Defocused Dark-Field Orientation Imaging of Single Gold Microrods on Synthetic Membranes

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Plasmonic gold microrods (AuMRs) are promising optical probes because of direct observation of their in-plane orientations and motions under an optical microscope. However, our understanding on the optical properties of AuMRs is still very limited at the single particle level and their out-of-plane orientations cannot be resolved by eye with high accuracy. Herein, we present the scattering properties of 1 μm -long AuMRs under defocused DF microscopy. Characteristic defocused scattering patterns of single AuMRs allowed us to resolve both in-plane and out-of-plane angles of single AuMRs. We further demonstrate the feasibility of using the defocused orientation imaging technique to track rotational motions and out-of-plane angles of single AuMRs on synthetic membranes.

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Code: ANAL.P-161

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Label-free Optical Biosensor Based on Chemical Interface Damping Using Gold-nanorods

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We studied the optical properties of gold nanorods using a darkfield microscope(DF) and a scanning electron microscope(SEM). The existing LSPR based biosensor was a method of sensing by the shift of the SPR peak when the target molecule was attached. However, the dielectric constant of the surrounding medium affects this sensing method. So, we propose a label-free plasmon-based biosensor that is sensitive to the adsorption of biomolecules without being disturbed by the dielectric constant of the surrounding medium. When thiol is attached to gold nanorods, wavelength shifts and FWHM (Full Width at Half Maximum) are increase. This is called chemical interface damping(CID). As the line width increases, sensing becomes possible without being affected by the dielectric constant. We propose a biosensing method based on CID by confirming the change of the optical characteristics according to the aspect ratio and the broadening of the plasmon line width of the rod-shaped gold nanoparticles by using three kinds of gold nanorods having different aspect ratios.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Effect of Adsorbate Electrophilicity and Spiky Uneven Surfaces on Single Gold Nanourchin-based Localized Surface Plasmon Resonance Sensors

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We present single particle studies on urchin-shaped gold nanoparticles for their use as localized surface plasmon resonance (LSPR) biosensors under dark-field (DF) microscopy. First, the LSPR wavelength of single gold nanourchins (AuNUs) was red-shifted as thiol molecules were attached onto the surface. AuNUs with sharp tips showed higher sensitivity for detecting thiol molecules than gold nanospheres (AuNSs) of similar size. Second, the degree of red shift was strongly affected by the electrophilicity of adsorbate molecules on the nanoparticle surface. Single AuNUs capped with 4-nitrothiophenol (4-NTP) strong electron withdrawing groups (EWG) caused a larger red shift than those coated with 4-aminothiophenol (4-ATP) strong electron donating groups (EDG). Last, real-time monitoring of molecular binding events on single AuNUs was performed. The LSPR peak was red-shifted and saturated after introducing 1 μM of 4-aminothiophenol. Therefore, single AuNUs were highly sensitive to changes in medium dielectric constant as well as the electrophilicity of attached thiol molecules. The results indicate that single AuNUs with sharp tips can be used to develop highly sensitive LSPR biosensors.

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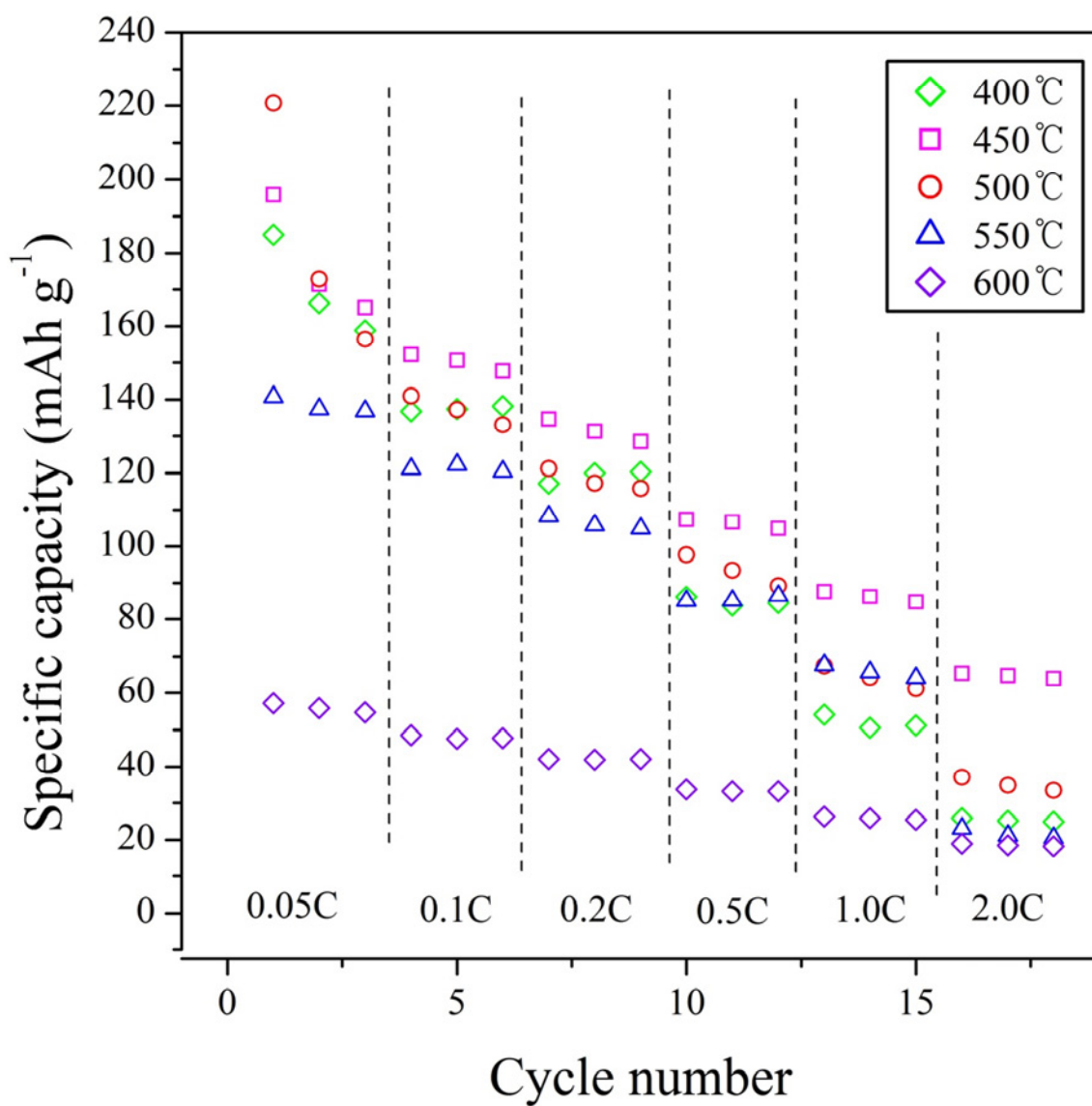
Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and characterization of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ cathode material prepared by a citric acid based sol-gel route

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A new cathode material, $\text{Li}_3\text{V}_2(\text{BO}_3)_3$, has been calcined by citric acid based sol-gel route at various temperatures ranging from 400 °C to 600 °C and characterized for optimization of calcination temperature. The $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ as cathode material for LIBs was investigated on electrochemical performances. Citric acid acts not only as a chelating agent but also as a carbon source, which enhance the conductivity of the composite material and hinder the growth of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ particles during preparation. The structure and morphology of $\text{Li}_3\text{V}_2(\text{BO}_3)_3$ were characterized by X-ray diffractometry (XRD) and scanning electron microscopy (SEM). Galvano-static charge/discharge and cyclic voltammetry (CV) measurements were used to study its electrochemical behaviors which indicate the reversibility of the lithium extraction/insertion processes. The sample synthesized at 450 °C exhibits the highest capacity of 198 mAh g⁻¹ at 0.05C and excellent cycle ability.



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Study of electrochemical properties for porous $\text{Li}_3\text{V}_2(\text{BO}_3)_3/\text{C}$ as a cathode material its characterization using MAS NMR for Li-ion batteries

Ji Won Lee, CHAEWON Moon, YOUNGIL LEE*

Department of Chemistry, University of Ulsan, Korea

Recently, poly-anion based compounds such as phosphates, silicates and borates as cathode materials for Li-ion battery have been developed for using in individual IT device, electric vehicles, and high energy storage systems have been investigated due to low cost and structural stability. Among these compounds, monoclinic $\text{Li}_3\text{V}_2(\text{PO}_4)_3/\text{C}$ (LVP) has good thermal stability, structure stability and the highest theoretical specific capacity of 197 mAh g^{-1} in the potential range of 3.0 – 4.8 V. However, LVP has low electronic conductivity and Li-ion diffusion coefficient (10^{-8} to $10^{-14} \text{ cm}^2 \text{ s}^{-1}$). So, we have attempted to fully exchange the phosphate to the borate in order to improve specific discharge capacity. This material has been synthesized by combustion synthesis method and the morphology, compositions and electrochemical performance of the synthesized sample were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Cycling test and Galvanostatic charge-discharge measurement and mainly analyzed the structure character using solid-state MAS NMR. As a result, we demonstrates the electrochemical performances of a highly porous $\text{Li}_3\text{V}_2(\text{BO}_3)_3/\text{C}$, synthesized via combustion synthesis as a new cathode material with a wide range voltage operability of 0.9 to 4.5 V which delivered exceptionally high discharge capacity 257 mAhg^{-1} at 0.05 C, 95.6% of its theoretical capacity.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Chromatographic Enantiomer Separation of Chiral Amines as Nitrobenzoxadiazole Derivatives on Several Polysaccharide-Derived Chiral Stationary Phases by Normal HPLC under Simultaneous Ultraviolet and Fluorescence Detection

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A convenient and derivatized method using a fluorogenic agent, 4-chloro-7-nitro-1,2,3-benzoxadiazole (NBD-Cl) was developed for enantiomer resolution of chiral aliphatic amines including amino alcohols by normal HPLC. The enantiomer separation of chiral amines as NBD derivatives was performed on six covalently bonded and four coated type polysaccharide-derived chiral stationary phases (CSPs) under simultaneous ultraviolet (UV) and fluorescence detection (FLD). Among the covalently bonded CSPs, Chiralpak IE showed the best enantiomer separation for most analytes. The other CSPs also showed good enantioselectivity except for Chiralpak IB. On the other hand, Chiralpak AD-H and Amylose-1 generally exhibited better enantiomer separation of NBD derivatized chiral amines among the coated CSPs. The developed analytical technique was also applied to determine the optical purity of commercially available (R)- and (S)-leucinol; the impurity was found to be 0.06%. The developed method was validated and proved to be an accurate, precise, sensitive and selective method suitable for enantiomer separation of chiral aliphatic amines as NBD derivatives under simultaneous UV and fluorescence detection.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Forensic Platform for Identification of Human Saliva using MS-based Glycomics

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In forensics, saliva found at crime scenes is one of the important evidences and thus, the identification of human saliva from other human fluids and non-human fluids, respectively is an essential prerequisite prior to further crime investigation. In previous study, we could determine that the degree and amount of highly fucosylated N-glycans were specific features to identify human saliva from other body fluids through MS-based glycomic approach. However, most saliva encountered at crime scenes has a trace amount and has been often found as a dry spot. For these reasons, forensic platform with high sensitivity for identification of human saliva is required. Herein, we have developed MS-based platform using glycomics and characterized N-glycans extracted from a trace amount of dried saliva. Briefly, dried saliva was prepared by spotting the saliva onto a protein saver card and drying at ambient temperature. N-glycans were enzymatically released by PNGase F from dried saliva spot (DSS) and enriched by solid phase extraction with a porous graphitized carbon cartridge. Then, saliva N-glycans were characterized by MALDI-TOF/TOF MS. N-glycans found in DSS showed a high correlation in terms of the number of glycans and their amount compared with N-glycans released from saliva fluid. Indeed, highly fucosylated N-glycans were also observed as a specific signature in DSS. We also examined technical validated reproducibility of N-glycan analysis based on DSS. This is the first study to apply a glycomic tool to forensic science.

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Area: Analytical Chemistry

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High-throughput Automated Platform for Native Glycan Analysis using Liquid Handling System

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Glycosylation of therapeutic glycoproteins is a key factor influencing biological function, safety, and protein stability. To assure quality of biopharmaceuticals, glycosylation should be analyzed at all stages of manufacturing process since it could be changed by cell culture and environmental conditions. For sample preparation, automated system is often necessary in pharmaceutical industry to reduce hands-on time and to obtain accurate and reproducible data. Here, we present the robotic platform to release and enrich glycans from glycoproteins by liquid handling system combined with 96-well microplate. Overall processes including protein denaturation by heating block, N-glycan release by PNGase F, and glycan enrichment by solid phase extraction (SPE) were automatically performed. Especially, the technical variation was mostly affected by PGC-SPE to purify and fractionate different types of glycans. For setting up SPE conditions, we used glycoprotein mixtures including diverse glycans which were eluted by varying proportions of acetonitrile in water and formic acid. Consequently, we obtained three eluents consisting of high-mannose and complex-type glycans w/wo sialic acid residues. Automated full steps for glycan preparation is being repeatedly performed to validate the technical reproducibility of our platform. Ultimately, it can be applied for monitoring bioactive glycans of biotherapeutics or clinical glycan biomarkers.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Molecular level characterization of chemical compounds in crude oil deposit from tanks in Artawi oil field (Iraq)

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Molecular level characterization to identify and measure the deposits from the petroleum fluids were performed. The crude oil deposit was obtained from tanks located at Artawi field in south of Iraq /Basrah. Separation by centrifuge and filtration were used to prepare the sample. The samples were fractionated into three layers (upper part deposit sticky, middle part water and lower part deposit soil). The chemical compounds in the crude oil deposit were characterized by using ultra-high resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) along with (+) mode atmospheric photoionization (APPI) and (-) mode Electrospray Ionization (ESI) ion source. FT-ICR MS analysis provides comprehensive heteroatoms class distribution. The deposit of crude oils yielded distributions of hydrocarbons and heteroatoms. The results of such analysis showed the hydrocarbons are more abundant in the oil deposit soil, while the crude oil and deposit of crude oil sticky showed the heteroatoms are more abundant than hydrocarbons. Therefore, these procedures provide an understanding of the overall behavior of the species that precipitate as well as of the interactions among those compounds.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Quantification of Inorganic Arsenic using Ion Exchange Membrane by Laser Induced Breakdown Spectroscopy

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The toxicity, bioactivity and mobility of arsenic are dependent on the chemical forms or species in which it exists. It is well known that the inorganic arsenic is more toxic than the organic arsenic. Inductively Coupled Plasma-Mass Spectrometry(ICP-MS) coupled with chromatographic technique has been used to perform the qualitative and quantitative determination of the arsenic species in various samples. However, it has been difficult to conduct a overall analysis due to matrix effects and took a long time to separate the arsenic species in various samples with the complex matrix. In this study, the solid phase extraction(SPE) membrane was used to separate inorganic arsenics, and those were detected by laser induced breakdown spectroscopy (LIBS). The samples were prepared using a buffer solution with phosphate buffer saline (pH 7.4) to separate arsenic species. The recovery efficiency of As(V) by LIBS was 96.9 %. NIST water CRM 1643f was used to validate the method for the determination of inorganic arsenics in a sample. The recoveries of As(V) and As(III) by LIBS were 98.9 % and 102.0 % respectively. The new speciation method by LIBS has labor and cost advantages for the quantitation of inorganic arsenic.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis, dispersion and tribological potential of alkyl functionalized graphene oxide for oil-based lubricant additives

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Graphene has been reported as an excellent lubricant additive for reducing adhesion and friction when coated on various surfaces as an atomically thin material with low surface energy. We have developed graphene oxide (GO) grafted with long alkyl chains to improve dispersion in oil-base lubricant as largely enhanced lipophilicity. Alkyl functionalized GO is synthesized by reacting NH₂-GO with alkylchloride (n=4, 8, 14) in ethanol under reflux, then 0.02 wt% of alkyl functionalized GO (FGO 4, 8, 14) are added into the base oil (PAG 0W40) and ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene are investigated by Fourier transform infrared (FT-IR), X-ray photoelectron spectroscopy (XPS) and scanning electron microscope (SEM), Transmission electron microscopy (TEM), X-ray Diffraction (XRD) and Raman spectroscopy. The tribological tests are performed with High frequency friction/wear Tester. The van der Waals interaction between the tetradecyl chains grafted on GO and the alkyl chains of base oil provided long-term dispersion stability so that the C14-GO showed better dispersion than C4-GO, C8-GO. The C14-GO also decreased both friction and wear considerably under the rubbing contacts between ball and disk.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Characteristics and electrochemical performance of silica coated carbon nanocoils composite as an anode material for lithium secondary batteries

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We have performed a study of a silica/carbon nanocoils (SiO₂-CNC) nanocomposite as a potentially high performance anode for rechargeable lithium secondary batteries. Carbon nanocoils were grown via chemical vapor deposition (CVD) method. Acetylene (C₂H₂) and Sulfur hexafluoride (SF₆) were flowed into the quartz reactor of a tubular furnace heated to 550 °C at 100 torr and maintained for 60 min to synthesize CNCs. CNCs were then put into the Tetraethyl orthosilicate (TEOS) to synthesize SiO₂-CNCs composite. The electrochemical characteristics of SiO₂-CNCs composites as an anode of Li secondary batteries were investigated using three-electrode cell. The SiO₂-CNCs composites loaded on Ni foam were directly employed as an working electrode without binder. As the counter and reference electrode used lithium foil. 1M LiClO₄ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC): ethylene carbonate (EC) in a 1:1 volume ratio. Glass fiber separator was used as the separator membrane. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. The morphologies, compositions and crystal quality of the prepared SiO₂-CNCs composites were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), energy X-ray diffraction (XRD), dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). As a result electrochemical performance of SiO₂-CNC was better than existing carbon nanofibers and carbon nanocoils.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

On-line proteolysis and glycopeptide enrichment using dual micro-scale porous polymer membrane enzyme reactor (μ PPMER) and nanoflow liquid chromatography-tandem mass spectrometry

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N-glycosylation is a type of glycosylation that occurs when glycans are attached to the nitrogen atom of asparagine (asn, N). It is important to analyze N-glycoproteins in biological samples as they play essential roles in protein folding or signaling process. However, analysis of glycoproteins from glycopeptides by shotgun analysis can be time-consuming and sample loss is inevitable during pre-treatments. Therefore, to overcome such problems, dual micro-scale thermo-sensitive porous polymer membrane enzyme reactors (μ PPMER) has been utilized for on-line proteolysis, followed by enrichment of glycopeptides prior to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS/MS). A thermo-responsive porous polymer membrane (T-PPM) was synthesized by coating PS-co-MAN-NIPAM polymer on bare nylon membrane and its characterization was conducted by SEM. Trypsin and lectin were immobilized on the coated membrane for proteolysis and glycopeptide capture, respectively, and each of membrane was inserted in μ PPMER module. Dual μ PPMER modules were connected to nLC-ESI-MS/MS system for on-line analysis and efficiency in glycopeptides enrichment selectivity under various temperatures were evaluated. In addition, glycoproteins from human plasma and urine samples were analyzed using on-line dual PPMER module in the most optimized condition for glycopeptide enrichment.

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Code: ANAL.P-173

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Effect of high fat diet on mouse brain lipidomes by nUPLC-ESI-MS/MS : Cortex, Hippocampus, Hypothalamus, & Olfactory bulb

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Lipids are known to be involved in various neuronal functions in brain, which is one of the most important and complex organ in the central nervous system. As brain plays a number of roles including cognition, memory, learning, and metabolic control, brain dysfunction can eventually lead to a variety of diseases. Recently, lipidomic analysis in relation to brain diseases has attracted much attention. High fat diet (HFD) can cause insulin resistance in the brain tissues by inducing obesity through diet. Although the effects of HFD on brain health have been studied in pathology, the relationship between HFD and brain lipid profiles has not been extensively studied. In this study, four different brain tissues (cortex, hippocampus, hypothalamus, and olfactory bulb) from mouse upon high fat diet programs have been analyzed using nanoflow ultrahigh pressure LC-ESI-MS/MS (nUPLC-ESI-MS/MS) for the investigation of HFD effect on the changes in the lipid profiles. Mice were fed with the various dietary plans: 8 weeks normal control (N), and weight gain (F), 16 weeks normal control (NNN), weight maintenance (FNN), weight gain (NNF), and weight cycling (FNF). As a result, 270 lipids including phospholipid, glycerolipid, and sphingolipid were quantified and statistical analysis was applied.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Analysis of HDL from coronary artery disease patients through bottom-up and top-down proteomic approach using flow field-flow fractionation and mass spectrometry

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Coronary artery diseases (CAD) is a disease caused by narrowing of the coronary arteries of the heart by plaque, fat or other substances. Narrow coronary artery interfere with blood flow to heart and may even cause damage in heart or eventually lead to death. High-density lipoprotein (HDL) has been reported to be associated with CAD as marker molecules. Lipoprotein is known as a macromolecules that transports lipids through the blood. These lipoproteins are divided into different classes depending on their density and specific role. HDL is composed of lipid and various proteins including apolipoproteins. One of the roles of HDL to transport excess cholesterol to the liver and regulate cholesterol levels in cells, blood vessels, and blood. Transportation of cholesterol by HDL helps to remove excessive cholesterol out of cells, blood, and blood vessel wall. Recent studies have been reported that apolipoprotein A-I in HDL goes through oxidation in severity of CAD. Flow field-flow fractionation (FIFFF) is widely used to separate macromolecules and nanoparticles according to their hydrodynamic diameter. In this study, HDL from human plasma of CAD patients was separated by FIFFF. Miniaturized asymmetrical FIFFF (AF4) channel was coupled on-line to electrospray ionization mass spectrometry (ESI-MS) for a high speed separation of lipoproteins and top-down proteomic analysis for various proteins including ApoA-1 from HDL were analyzed in order to investigate the change in HDL-related proteins caused by severity of CAD.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Steric Transition Phenomena upon Field Decay Patterns Using Frit-inlet Asymmetrical Flow Field-Flow Fractionation

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Flow field-flow fractionation (FIFFF) is a separation technique that can separate macromolecules by size without stationary phase. The separation mode of FIFFF can be divided into normal and steric/hyperlayer mode; particles with sizes smaller than 1 μ m are operated in normal mode while those larger 1 μ m are operated in steric/hyperlayer mode. During the focusing/relaxation process, smaller particles diffuse more and equilibrate at a position higher from the channel than larger particles. As a result, The smaller particles are located in faster flow stream and eluted earlier than the larger particles. In the steric/hyperlayer mode, where the particle size is larger than 1 μ m, Brownian diffusion becomes negligible and particles are elevated to a certain height by lift force. Since the larger particles have higher lift forces than the smaller particles, they elute earlier. Steric transition is a phenomenon that particle elutes by a combination of normal mode and steric mode in FIFFF. Frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) operates by stopless flow without focusing process. In this study, steric transition phenomenon is systematically monitored with polystyrene particles by FI-AF4 coupled with UV/visible detector and multi-angle light scattering. Depending on the strength and gradient of the field, the particle size at which the steric transition occurs varies. Therefore, it is possible to increase the range of particle size separated in the normal mode.

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Profiling of lipoproteins from patients with mild cognition impairment and Alzheimer's disease by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

SAN HA KIM, JoonSeon Yang, Myeong Hee Moon*

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Recently, as the average life span of people is increasing, the number of elderly population has been rising sharply and cognitive impairment disorders with aging factor such as Alzheimer's disease have become common. Amyloid-beta plaques is known to be a major cause of Alzheimer's disease and kills neighboring brain cells, which leads to dysfunction in cognitive abilities. Symptoms of Alzheimer's disease's are usually developed decades after the accumulation of amyloid-beta. Therefore, the rate of disease progression is even faster when symptoms start to appear. About 10 percent of patients with mild cognitive impairment, a pre-stage of Alzheimer's disease, end up diagnosed with Alzheimer's disease within a year. Several studies have reported that high levels of low-density lipoprotein(LDL) and low levels of high-density lipoprotein(HDL) is affected amyloid-beta. Therefore, it is important to understand lipid metabolism from separating HDL and LDL, separately. In this study, lipids from human plasma samples of healthy controls, patients with mild cognition impairment, and Alzheimer's disease patients were analyzed. Lipoproteins were fractionated by asymmetrical flow-field flow fractionation and the lipids were extracted from the collected fractions of HDL and LDL and structurally identified from collision-induced dissociation of nanoflow ultrahigh-pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS). More than 300 lipids were identified. Identified lipids are quantified from individual samples to evaluate the difference between the two groups in comparison to those of healthy controls.

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Lipidomic analysis of blood plasma from patients among five different cancer types by nUPLC-ESI-MS/MS

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As lipids are associated with functions such as chemical-energy storage, cellular signaling, cell membranes, and cell to cell interaction, they play a key role in cellular survival, proliferation, and death. These cellular processes are vitally concerned with carcinogenesis pathways, especially to transformation, progression, and metastasis, suggesting the bioactive lipids are mediators of a number of oncogenic processes. According to recent lipidomics research, lipid analysis regarding cancer is very important, since each type of cancer has different carcinogenesis pathways. In this study, lipids from plasma of healthy controls and patients with cancers (liver, stomach, lung, colorectal, and thyroid) were investigated in order to discover lipids that show significant difference between the groups and find potential lipid biomarkers for each cancer. Blood plasma were extracted from each control and cancer patients using the modified Folch method with MTBE/methanol, and the extracted lipids were analyzed by nLC-ESI-MS/MS. A total of 243, 236, 239, 239, 239, and 225 lipids from plasma of patients with liver, stomach, lung, colorectal, thyroid cancer, and controls, respectively, were identified and profiling of lipid from each case of cancer was compared with that of controls.

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An investigation on the various internal standards for the accurate determination of the arsenic species in rice

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Rice is a staple food in the world's half population and is a major source of human arsenic intake. But, toxicity of arsenic depends on its chemical forms. Therefore, the selective and quantitative determination of the total arsenic as well as the arsenic species in rice has been very important. However, the extraction and determination of arsenic species in rice has been very difficult because of the severe matrix interference. In this study, the various analytical methods including the internal standard method and standard addition method have been investigated for the determination of arsenic species in rice. The extraction solvent has been used 0.28 M nitric acid. A new analytical method was developed for the determination of arsenic species in rice by inductively coupled plasma - mass spectrometry (ICP-MS) coupled with ion chromatography (IC). Rice certified reference material (NIST SRM 1568b rice flour) was used to evaluate its suitability for the analytical method. In this study, two internal standards were used. The first internal standard was injected before sample introduction to correct the signal change with time, and the second internal standard was spiked into the sample to remove or reduce the matrix interferences. Recoveries of inorganic arsenic, DMA, MMA, and total arsenic for the certified values were 92 %, 116 %, 107 % and 107 %, respectively, with the developed method.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

LC-MS/MS determination and pharmacokinetic study of Sorafenib in rat and beagle plasma

yoojeong yoon

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A rapid, sensitive and selective liquid chromatography/tandem mass spectrometry method (LC-MS/MS) has been developed and validated for the identification and quantification of Sorafenib in rat and beagle plasma using Sorafenib-d3 as an internal standard. Sample pretreatment involved simple protein precipitation (PPT). Chromatographic separation was carried out on a poroshell 120 EC-C18 column (3.0 × 50mm, 2.7 μm, Agilent) at 35 °C using an isocratic elution method with acetonitrile/0.1% formic acid in 10mM ammonium formate: 70/30 (v/v) at a flow rate of 0.2mL/min. Detection was performed using electrospray ionization in positive ion multiple reaction monitoring (MRM) mode by monitoring the ion transitions from m/z 465.3 → 252.2 (Sorafenib) and m/z 468.1 → 255.0 (internal standard). Calibration curves were linear in the concentration range of 5–5000 ng/mL. The overall precision and accuracy for all concentrations of quality controls and standards were better than 15%. The validated method was successfully applied to the pharmacokinetic study of Sorafenib in rat and beagle plasma..

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-180

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Characterization of Graphene-enfolded TiO₂ Anatase as Anode Materials for Li-Secondary Batteries

Hasan Jamal

Department of Chemistry, Keimyung University, Korea

In this study, graphene-bonded and enfolded anatase TiO₂ of various types composites have been synthesized without using any cross-linking reagent, by using graphene oxide (GO) and titanium dioxide as a precursor. In which graphene sheets are uniformly dispersed among the TiO₂ anatase particles, in order to enhance the cyclic ability and electronic conductivity of TiO₂ anode for lithium ion batteries. The composites of GO with three types of anatase TiO₂ (Nanoparticles, Nanorods, Nanofibers) were synthesized by hydrothermal and calcination treatment. The reduction of GO was simultaneously proceeded after the calcination in an argon atmosphere at 400 °C for 4 h. The physicochemical properties were characterized by Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. Surface properties were measured by BET & BJH method. The electrochemical properties were also investigated by cyclic voltammetry (CV) and Electrochemical Impedance Spectra (EIS). The TiO₂ nanorods/graphene composite having unique morphology showed superior discharge capacity of 135 mAh g⁻¹ at a current density of 0.5 C than other types of TiO₂ composites and achieved a reversible capacity of 105 mAh g⁻¹ after 35 cycles.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ANAL.P-181**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Quantitative analysis of residual lactide in Polylactide by NMR and GC

HYERIM KIM

Samyang Biopharmaceuticals Corp., Analytical Science Center R&D Center, Korea

Poly(lactide)(PLA) is one of the biodegradable aliphatic polyesters and has been widely applicable in the field of bio-medicine and environmentally friendly products. Industrially, PLA is produced by ring-opening polymerization of lactide in bulk, and purified through de-volatilization at high temperature under high vacuum. The performances of PLA are directly affected by the content of residual monomer in polymers, such as having harmful effects during processing and also causing undesired property changes in the end products, lowering mechanical strength and thermal stability, and increasing the hydrolytic degradation rate of PLA products. In this study, We have developed methods to quantitatively determine the residual lactide monomer in PLA using NMR spectroscopy compared with conventional gas chromatography(GC) methods. There was no significant difference in the results of quantification of the residual lactide monomer in PLA by NMR and GC. So, NMR spectroscopy can be a powerful tool for the analysis of residual lactide.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ANAL.P-182**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Equipment for lung cancer diagnosis via breath analysis using IMS

HeeJin Moon

R&D, Sensor Tech, Korea

As lung cancer in its progress has no major symptoms other than coughing and phlegm, it is hard to diagnose, and also it has the highest mortality rate compared to other cancers, so early diagnosis and treatment is very important. This research is to develop a non-invasive device to diagnose lung cancer early which utilizes ion mobility spectrometry (IMS) to analyze exhaled breath. Early diagnosis can be achieved by analyzing the change in specific biomarkers found in exhaled breath of lung cancer patients out of various volatile organic compounds (VOCs) in exhaled breath. The device in this research is convenient, highly sensitive, provides fast analysis and low false diagnosis. The device aims to lower lung cancer deaths and lower the society's economic burden caused by lung cancer.

120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

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Code: **ANAL.P-183**

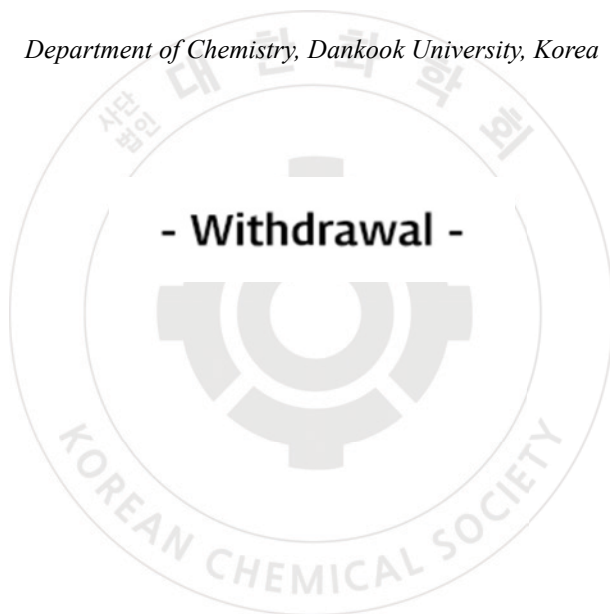
Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

**[Withdrawal] Study on boron analysis of NCM Anode active material
in lithium ion battery by ICP-MS**

In Gi Kim, Heung Bin Lim^{*}

Department of Chemistry, Dankook University, Korea



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL.P-184

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Optimization of sample preparation for the identification of GB-tyrosine in rat plasma exposure to GB

JIHYUN KWON, Yong Gwan Byun, Yong Han Lee*

Agency for Defense Development, Korea

The identification of the chemical warfare agent, isopropyl methlyphosphonofluoridate (sarin, GB) in plasma has been studied using liquid chromatography-tandem mass spectrometry (LC-MS/MS). However, systematic study of sample preparation for LC-MS/MS was not done a lot. Therefore, the sample preparation for the identification of GB-tyrosine in rat plasma was studied. Also, the lowest detection concentration of GB-tyrosine for LC-MS/MS was reported using the optimized sample preparation. The optimized sample preparation will be employed to study other types of nerve agent in plasma.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ANAL.P-185**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Anti aging effect of green tea extract and its application to the herb material of emulsion base

Young Jun Park

Cha university, Korea

Jeju island is located at the south area of Korean peninsula. It has a natural resources of wild grown herbal medicine plants. Various species currently classified as herbs are grown or cultivated in Jeju. Recently, studies on catechin have attracted interest to control wrinkles aging on skin man and woman. The proposal of this study was to determine whether catechin compound mixture, the active ingredient, could be used as herbal extract to improve aging wrinkles, especially for middle aged group using various test. First, this study determined its elastase activity and anti oxidizing effect by DPPH assay in vitro, to evaluate the efficacy of emulsion catechin prototypes in improving anti aging. This study will provide basis for the development of catechin prototypes with advanced composition technology. It will add a step forward to the herbal cosmetic industry.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-186

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Quantum Dot Dissolution Based Electrochemical Immunosensor for a Post Mortem Interval Biomarker Detection in Serum Sample

BongJin Jeong, RASHIDA AKTER, Jeonghyun Oh, Md. Aminur Rahman*

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

In the present work, an electrochemical post mortem interval biomarker immunosensor was fabricated on the and quantum dot (QD) attached graphene oxide (GO) incorporated cysteamine (Cys) self-assembled monolayer (SAM) based platform for the detection of glyceraldehyde 3-phosphate dehydrogenase (GAPDH) in human serum sample. Monoclonal anti-GAPDH antibody was covalently immobilized on the carboxylic acid functionalized cadmium selenide (CdSe) QD through the amide bond formation by EDC/NHS coupling. The immunosensor surface was characterized using scanning electron microscopy (SEM) and energy The GAPDH detection was made through the dissolution of the surface attached CdSe QD by glucose oxidase (GOx) enzyme generated hydrogen peroxide, which was used as an enzymatic label. For enhancing the sensitivity, we performed the competitive assay in which GD-GOx conjugates and free-GD competed for binding to the active sites of antibody. The current response resulted from the optimized CdSe dissolution was found to be decreased with increasing concentration of free GD and was proportional to the free-GD concentration. Differential pulse voltammetry (DPV) technique was used to determine the analytical characteristics such as detection limit (DL), linear dynamic range, selectivity, stability, and the real sample analysis for the GD detection. The proposed GAPDH immunosensor showed a wide linear range from 1.0 fg / mL to 100 ng / mL and exhibited a low detection limit of 2.0 fg / mL. The practical application of the immunosensor was tested in the human serum samples, which can be used in the forensic science field.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-187

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Graphene Oxide/Polytyramine Nanocomposite Based Immunosensor for Electrochemical Protein Detection

MD. ARIF-UR RAHMAN, RASHIDA AKTER, BongJin Jeong, Jeonghyun Oh, Md.

Aminur Rahman*

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

The sensitive detection of a serum cytokine protein, interleukin-6 (IL-6) was carried out using a polytyramine/graphene oxide/ (Ptyr/GO) nanocomposite film based electrochemical immunosensor. Monoclonal anti-IL-6 antibody was covalently immobilized on the Ptyr/GO nanocomposite film through the covalent bond formation between the amine groups of Ptyr and antibody through the glutaraldehyde crosslinking. Magnetic bead (MB) supported numerous thionine (Th) labels were used for the sensitive detection of IL-6 through the electrocatalytic reduction of hydrogen peroxide (H₂O₂). The GO/Ptyr immunosensor surface was characterized using cyclic voltammetry (CV), scanning electron microscope (SEM), electrochemical quartz crystal microbalance (EQCM), and electrochemical impedance spectroscopy (EIS) techniques. Square wave voltammetric (SWV) technique was used to measure the electrochemical response after optimizing the experimental conditions. The proposed Ptyr/GO nanocomposite based immunosensor with MB-supported Th labels showed a low limit of detection (LOD) of 0.1 pg/mL and wide linear range between 0.5 and 100 pg/mL with excellent stability and enhanced selectivity. The detection ability of the proposed immunosensor was compared with an enzyme-linked immunosorbent assay (ELISA) method and was applied to various IL-6 spiked human serum samples.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-188

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Improving Electrochemical Protein Detection through Enhancing Biocatalyzed Precipitation Using Bienzymes Coated Carbon Nanotubes

RASHIDA AKTER, MD. ARIF-UR RAHMAN, Jeonghyun Oh, BongJin Jeong, Md. Aminur Rahman *

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

A highly sensitive electrochemical detection of mucin 16 (MUC16) based on enhanced biocatalyzed precipitations using bienzymes glucose oxidase (GOx) and horseradish peroxidase (HRP) coated multiwall carbon nanotubes (MWCNTs) was developed for the early diagnosis of ovarian cancer. The immunosensor was fabricated by covalently immobilizing monoclonal anti-MUC16 antibody on noncovalent functionalized graphene oxide (NGO) on gold nanoparticles (AuNPs) modified indium tin oxide (ITO) electrode (immunosensor probe). The MUC16 (target protein) and anti-MUC16/MWCNTs/GOx/HRP conjugate were bonded with the immunosensor probe through the immunoreaction. The biocatalyzed precipitation of 4-chloro-1-naphthol (CN) by bienzymes was then carried out at the immunosensor probe. The insoluble precipitates accumulated on the immunosensor probe and acted as a barrier for the direct electron transfer (ET) reaction of an external Fe(CN)₆³⁻/Fe(CN)₆⁴⁻ redox couple. The amplified detection was achieved through the increased ET blocking ability of the immunosensor by numerous precipitates using enormous numbers of GOx and HRP on MWCNT and the in situ generation of an enzymatic substrate, hydrogen peroxide (H₂O₂). The immunosensor surface was characterized using scanning electron microscope (SEM), quartz crystal microbalance (QCM), and electrochemical impedance spectroscopy (EIS) techniques. Cyclic and square wave voltammetric techniques were used to monitor the electrochemical responses before and after precipitation reaction. Under the optimized experimental condition, the proposed immunosensor with bienzymatic label showed a low limit of detection (LOD) and wide linear range, which were 10 times lower and wider than those obtained for an immunosensor with a single enzyme (HRP) label. The validity of the proposed method was compared with an enzyme-linked immunosorbent assay (ELISA) and was applied to various MUC16 spiked human serum samples for the selective detection of MUC16.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-189

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Simultaneous Multiplexed Detection of Multiple Cancer Biomarkers using Graphene Oxide Electrode Array and Metal Ion Tagged Dendrimer Label

RASHIDA AKTER, BongJin Jeong, Md. Aminur Rahman*

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

The simultaneous multiplexed detections of three prostate cancer (PC) biomarkers, prostate specific antigen (PSA), prostate specific membrane antigen (PSMA), and interleukin-6 (IL-6) were carried out using a triple graphene oxide electrodes array on indium-tin oxide (ITO) and metal ion tagged dendrimer labels. To fabricate the immunosensor array, three monoclonal antibodies, anti-PSA, anti-PSMA, and anti-IL-6 were covalently immobilized on the three separate 1-pyrenecarboxylic acid (Py-COOH) functionalized GO modified ITO surface using EDC/NHS coupling. Three different types of metal ions such as Cu^{2+} , Cd^{2+} , and Zn^{2+} were coordinated with a third generation dendrimer with 32 surface terminated carboxylic acid groups through 5-aminoisophthalic acid, which were conjugated with three different types of antibodies. In the presence of the specific biomarker such as PSA, PSMA, and IL-6, the anti-PSA, anti-PSMA, and anti-IL-6 antibodies conjugated metal ions tagged dendrimer label attached to the immunosensor arrays. The multiplexed detection of three different types of biomarkers were achieved through directly monitoring the stripping current of the metal ions without any harsh acid dissolution step. Linear sweep voltammetric (LSV) technique was used to measure the stripping currents of respective metal ions in acetate buffer at pH 4.6 after optimizing the experimental conditions. The present immunosensor array exhibited low limit of detections (LODs) and wide linear ranges for three prostate cancer biomarkers with excellent stability and improved selectivity. The applicability of the proposed multiplexed immunosensor array was verified by comparing the immunosensor results with individual enzyme-linked immunosorbent assays (ELISA) for PSA, PSMA, and IL-6 was successfully tested to human serum samples for practical applications.

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Venue: Kimdaejung Convention Center, Gwangju

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Silicon-Coated Gold Nanoparticle for Dual Imaging and Therapy

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¹*Department of Chemistry, Hanyang University, Korea*

²*Department of Advanced Materials Engineering, The University of Suwon, Korea*

Gold nanoparticles (Au NPs) have been used as effective Surface-Enhanced Raman Spectroscopy (SERS) substrates for decades. We synthesized the Au NPs through seeded growth method using a sodium citrate as stabilizer and reducing agent. However, this citrate-stabilized Au NPs become unstable when the environment changes abruptly, and agglomeration and sedimentation usually occur because of the properties of the stabilizers on the Au NPs surface. Therefore, improving the stability of Au NPs has important significance. At present, there are many coating methods to stabilize the Au NPs, such as silver, alumina and so on. However, one such robust functionalization that has been proven to enhance gold nanoparticle stability both thermodynamically and chemically is silica coating. The synthesis of Au NPs and silica coating were confirmed by UV spectroscopy, SEM, and TEM. In addition, we converted m-SiO₂ to mesoporous silicon (m-Si) by using magnesiothermic reduction. Si can make an amplified signal by DNP, one of the hyperpolarization phenomena, so that it can be used for MR imaging probe. Consequently, silicon-coated gold nanoparticle (Au NPs@Si) can be used for dual imaging, SERS and MR imaging. Moreover, Au NPs have been used for thermal therapy for cancer as photo-thermal agents for a long time and mesoporous silicon can be used for drug delivery. Therefore, Au NPs@Si can be used for dual therapy, both thermotherapy through the Au NPs and chemotherapy through mesoporous silicon. As a result, we developed Au NPs@Si as the probe for dual therapy and dual imaging for cancer diagnosis and therapy.

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Code: ANAL.P-191

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Porous Silicon and Carbon Nano-spheres as Hyperpolarized MRI Probes for Cancer Diagnosis

DOKYUNG KIM, Ikjang Choi, Youngbok Lee*

Department of Bionano Technology, Department of , Korea

Silicon and carbon based nano-spheres have been attracting a lot of interest in the field of biomedical applications due to their biocompatibility and biodegradability in vivo, as well as their flexible surface modifications. Here, we synthesized and investigated porous silicon (PSi NPs) and carbon nano-spheres (CNS) as hyperpolarized MR imaging probes. The Si NPs and CNS have many great benefits to the hyperpolarized MR imaging. Since core regions of the crystalline nano-spheres are mostly protected from a main relaxation source, such as paramagnetic centers existing at surface defect sites, these nano-spheres show extremely long depolarization times (usually longer than 30 mins), resulting in high MR image contrast with minimum or no background signals. In addition, paramagnetic centers on the surface defect sites play a pivotal role in generating MR signal enhancements induced by dynamic nuclear polarization (DNP) processes, thereby not necessary to add external radical sources. Two different synthetic approaches were demonstrated in order to produce PSi NPs and CNS. (1) Magnesiothermic reduction of porous silica (synthesized by modified stöber method with CTAB template) was processed in order to yield PSi NPs. (2) CNS was synthesized through the polymerization process of dopamine. Several spectroscopic and microscopic results suggest that the synthesized PSi NPs and CNS can potentially be utilized as biocompatible and targetable contrast agents for hyperpolarized MRI researches.

Conference Date: October 18~20, 2017

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Code: ANAL.P-192

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Determination of Fenpyroximate from Honey by LC-MS/MS

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Fenpyroximate is one of the insecticides used in beekeeping farms. This may remain in honey, which is regulated and banned in some countries. Honey have a complex matrix and therefore, it proceeded by combining Liquid-Liquid Extraction (LLE) and Solid Phase Extraction (SPE) for clean-up and concentration. The parameters for clean-up and concentration of the sample were optimized and validated. The parameters such as pH of sample, type of SPE cartridge, volume of extraction solvent, sample volume, volume of elution solvent, type of elution solvent were evaluated. were optimized. The chromatographic separation by LC-MS/MS system was achieved on an InfinityLab Poroshell 120 EC-C18 (3.0 mm i.d. × 50 mm length, 2.7 μm particle size) column using isocratic elution with water and acetonitrile (30:70). Ionization of the analyte was done by electrospray ionization (ESI) and quantitation was performed by multiple reaction monitoring (MRM). The limit of detection (LOD) and limit of quantitation (LOQ) from the spiked sample were 1.56 and 5.00 μg/kg respectively. The accuracy and precision in the working range (5.00-50.0 μg/kg) were 87.99-119.06 % and 0.68-14.29 % (RSD), respectively. The correlation coefficient (r^2) for the linear equations was obtained in the range of 0.9914-0.9977. The established method was applied to monitor thirty types of commercially available honey.

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Code: ANAL.P-193

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Analytical Platforms Employing LC-MS for Glycosylation Assessment of Therapeutic Glycoprotein

Nayoung Yun, Myung Jin Oh, Hyun Joo An*

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

Glycosylation of a therapeutic protein can significantly affect drug's stability, immunogenicity, PK/PD, and bioactivity. Therefore, glycomic analyses are necessary to assess biotherapeutic quality and biosimilar similarity. Current glycome analyses involve the use of complementary methods for assessing specific glycosylation attributes including glycan composition and structure, abundance, and glycosylation site with microheterogeneity. Here, we demonstrated a stepwise approach using MS platform for glycomic characterization, namely glycan analysis by glycomic approach, site-specific analysis using glycoproteomic approach, and intact protein analysis. Two representative therapeutic glycoproteins, interferon-beta-1a (IFN- β 1a) and trastuzumab, were used to compare the performance (results) of different analytical platforms. Interferon- β 1a (IFN- β 1a) possessing single N-glycosylation site was used for this study. IFN- β 1a and trastuzumab were prepared and analyzed using three independent analytical platforms. First, in intact protein analysis, the standards were desalted using 10K MWCO filters. Without further purification or enrichment IFN- β 1a was directly injected onto the nano LC C8 chip/Q-TOF MS. For glycopeptide approach, the standards were digested with pronase E and enriched and fractionated according to size and polarity by graphitized carbon solid phase extraction (GCC-SPE). In parallel, N-glycans were released from therapeutic proteins by PNGase F and then selectively enriched by GCC-SPE. The enriched glycopeptides and glycans were chromatographically separated and analyzed by nano LC PGC chip/Q-TOF MS, respectively. Regardless of analytical platforms, glycosylation profiling in both qualitative and quantitative analysis showed high correlation ($R=0.91\sim0.99$). Each platform showed different strengths and weaknesses, providing different levels of information on glycosylation. The results would be used as the reference for stepwise glycomic characterization during the development & production stage of biotherapeutics.

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Code: **ANAL.P-194**

Area: Analytical Chemistry

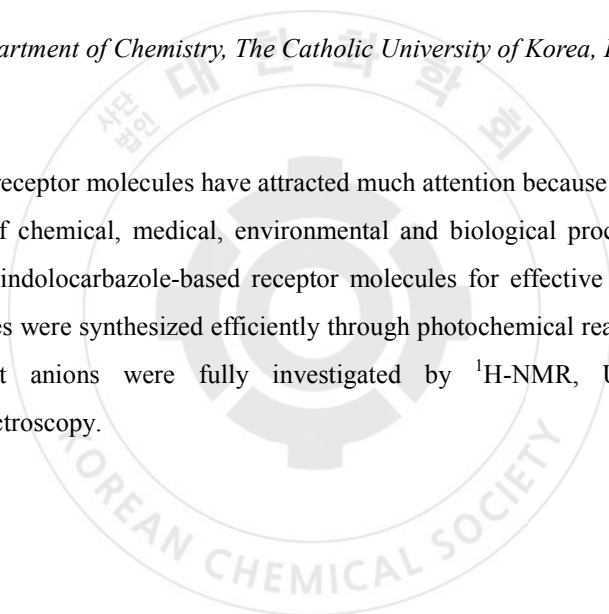
Type: Poster Presentation, Time: THU 11:00~12:30

Indolocarbazole-Based Receptors: Synthesis, Characterization and Anion Sensor Applications

SeungYun Baek, Byeong-Kwan An*

Department of Chemistry, The Catholic University of Korea, Korea

Recently neutral anion receptor molecules have attracted much attention because anions play an important role in a wide range of chemical, medical, environmental and biological processes. In this study, we report a new series of indolocarbazole-based receptor molecules for effective anion sensing. The new anion receptor molecules were synthesized efficiently through photochemical reactions, and their abilities to recognize different anions were fully investigated by $^1\text{H-NMR}$, UV/vis absorption and photoluminescence spectroscopy.



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Area: Analytical Chemistry

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Phytochemical, Pharmacological and Cytotoxic Characteristics of a Bioactive Compound Isolated from the Aerial Part of *Stenochlaena palustris* Bedd

Adhikari Suraj, Wonjae Lee*

College of Pharmacy, Chosun University, Korea

The ethanolic extract of *Stenochlaena palustris* Bedd. (Blechnaceae) was investigated for phytochemical, pharmacological and cytotoxic properties in a dose-dependent manner. The gummy concentrate obtained from ethanolic extraction was designed as crude extract with a yield of 17.6% for investigation. Phytochemical study revealed the presence of glycosides, flavonoids, saponines and alkaloids. The antioxidant property was evaluated by both qualitative test (using thin layer chromatography) and quantitative test (DPPH scavenging assay, total phenolic content assay, total flavonoid content assay, total tannin content assay, reducing power assay, nitric oxide scavenging assay, hydrogen peroxide scavenging activity, hydroxyl scavenging activity). In the quantitative assay, the extract showed dose-dependent free radical scavenging activity ($IC_{50} \sim 30.5 \mu\text{g/mL}$) which is comparable to that of standard ascorbic acid ($IC_{50} \sim 7.08 \mu\text{g/mL}$). Analgesic activity was investigated on Swiss Albino mice by hot water tail immersion method where extract at dose of 200 mg/kg and 400 mg/kg exhibited significant ($P < 0.05$ and $P < 0.001$, respectively) inhibition of pain by 157.27 and 146.15 after 120 and 180 minutes respectively while the standard drug Diclofenac Na inhibition was found to be 217.67 after 180 minutes at a dose of 25 mg/kg body weight. A linear correlation was found between mortality rates of brine shrimp with increased sample concentration in cytotoxicity test. The results tend to suggest that the plant contains active constituent(s) responsible for the mentioned activities and supports the traditional uses of this plant which also require further investigations to isolate bioactive compounds and to identify its underlying mechanisms.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Electrochemical immunoassay for amyloid-beta 1-42 peptide in biological fluids interfacing with a gold nanoparticle modified carbon surface

Hye Jin Lee^{*}, Kyung Min Kim, Suhee Kim

Department of Chemistry, Kyungpook National University, Korea

In this poster, an electrochemical immunosensor involving the formation of a surface sandwich complex on a goldnanoparticle (NP) modified screen printed carbon electrode (SPCE) is demonstrated for the femtomolardetection of amyloid-beta 1-42 peptide(A β) in both serum and plasma. Both bioreceptors forming the assay are highly selective antibodies for A β , namely antiA β and which possess different binding sites for the Apeptide. In order to improve the sensing performance for complex biological fluidic matrix analysis, different mixed monolayers of thiol modified polyethylene glycol (PEG) and mercaptopropionic acid (MPA) were self-assembled onto the Au NP-SPCE followed by tethering antiA(12F4)to MPA using a heterobifunctional cross linker.

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Code: ANAL.P-197

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Detection of lung cancer biomarkers using sandwich assay based on surface plasmon resonance

Sang Hyeok Lee, Hye Jin Lee^{*}

Department of Chemistry, Kyungpook National University, Korea

In this poster, a surface sandwich sensing platform with surface plasmon resonance (SPR) technique is demonstrated to detect lung cancer biomarkers. To quantitatively analyse lung cancer biomarker, sandwich assay platform was developed. Detection was performed via lung cancer biomarkers onto a gold chip surface by the covalent linking, and then the subsequent binding material was followed for SPR sensing. We predict that our method can be further applied to the detection of a number of cancer biomarkers in biological samples.

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Code: **ANAL.P-198**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Analysis of defect mechanism using Micro-IR

young woong Ahn

Research Team of Total analysis, KCC Central Research institute, Korea

The FT-IR method is fast, sensitive and has the advantage of not being difficult to sample. In addition, the equipment is easy to operate and can be applied to various fields such as chemical structure analysis, quantitative analysis and reaction analysis by attaching various attachments. In the case of Micro-IR, a high-resolution microscope can be mounted on the IR to be used for defect analysis such as garbage and Cratering of coating specimens, analysis of impurity substances in fine areas, image mapping, and interlayer composition analysis of multi-layer structures. In this study, various defective specimens were analyzed and the causes of defects were identified and classified by type. Defects caused by foreign matter, contamination transfer, and film loss were detected the most, and it was confirmed that analysis of the interlayer composition was possible by analyzing the specimen of multi-layer structure

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Code: **ANAL.P-199**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Study on corrosion mechanism and temperature profile of painted specimens by salt spray test (SST)

JAEHEE KIM

Analysis Team, KCC central research institute, Korea

The purpose of this study was to identify the corrosion mechanism of painted steel sheets and to examine the change of temperature. In order to carry out the experiment, the painted steel sheet was prepared as a test group, and each specimen was corroded under different temperature conditions and observed with a Scanning Electron Microscope with Energy Dispersive Spectroscopy (SEM/EDS). However, it is difficult to observe the experiment in the general environment, because the corrosion rate is slow. So we set up the experiment to be smooth through two methods. First, scribe was applied to the specimens to the same extent so that the corrosion reaction proceeded faster. Second, the experimental environment was set so that salt water was sprayed at a constant pressure and speed using a SST (Salt Spray Test) analysis machinery. Through this experiment, it is possible to observe the corrosion reaction and the change stage, and to understand the relationship between temperature and corrosion degree.

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Code: ANAL.P-200

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

On-Chip Direct Diagnostics based on Grating Coupling of Scattered Nanometals in Evanescent Field Layer

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The grating coupling of a scattered novel nanometals was effectively utilized for direct diagnosis of influenza virus without amplification process. Gold nanopad was used as a substrate for analyzing hybridization of single-stranded DNA (ssDNA) with nanometal tag (silver) by total internal reflection scattering (TIRS) microscopy. The grating separated the scattering signals of the nanotag from that of the substrate and displaced the optical path of the scattered signals to avoid errors caused by numerous acquisitions. This sandwich hybridization based biosensor quantified the target until zeptomolar concentration without interference of background by grating associated TIRS. The detection method is a significant advance in the development of an amplification-free biosensor to greatly reduce the time of sample pretreatment for quantitative screening of influenza A (H7N9) virus.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-201

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Analysis of Famphur in Honey by Solid-Phase Extraction and GC-MS

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Famphur which is a highly hazardous pesticide classified by WHO, may have adverse effects on humans and environments. But there was no guideline for famphur remaining in honey. In this study, a method for the selective determination of famphur in four kinds of honey using solid-phase extraction(SPE) and gas chromatography-mass spectrometry(GC-MS) was established. 5 g of honey was dissolved in 10 mL of water and transferred to a C18 cartridge preconditioned with ethyl acetate and water. After washing with 2 mL of purified water, and then famphur was eluted with 6 mL of ethyl acetate and determined by gas chromatograph with mass spectrometer(GC-MS). Optimization of solid-phase extraction(SPE) parameters was evaluated by the pH of the sample, the type and volume of the elution solvent. Chromatographic separation was achieved on DB-35MS column(30 m × 0.20 mm × 0.33 μm), and oven temperature was raised from 120 °C to 310 °C at a rate of 25 °C/min, and then maintained for 2 minutes. The injection mode was the split mode(10:1), and m/z 218.0 was used as the quantitative ions in SIM mode. From the established extraction and GC-MS conditions, the limit of detection(LOD) and limit of quantitation(LOQ) in the spiked sample were 2 ng/g and 5 ng/g, respectively. Recovery studies were performed at 5 ng/g, 10 ng/g, 20 ng/g of fortification levels, and accuracy and precision in working range were 63.7-118.4 % and 1.0-27.7 RSD %, respectively. The calibration curves for the quantitative analysis were obtained the concentration range of 5~50 ng/g with correlation coefficients(R²) from 0.9883 to 0.9958. The proposed method was applied to the analysis of famphur in domestic honey samples.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ANAL.P-202**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Changes of Saliva N-glycome after Death: A Proof-of-Concept Study for Determining Time of Death

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The estimation of time since death (TSD) is the crucial part for investigations of the suspicious death in forensic science. However, standard methods of TSD estimation are easily confounded by extenuating circumstances and/or environmental factors. Therefore, a panel of TSD markers obtained from more acceptable and accurate method is necessary to definitely determine the time of death. Saliva, one of the vital fluids encountered at crime scenes, contains various glycoproteins which are highly affected by biochemical environment. Here, we investigated saliva N-glycans between live and dead rats to determine the alteration of N-glycans using animal model system due to the limitation of saliva collection from recently-deceased humans. Rat saliva samples were collected both before and after death. N-glycans were enzymatically released by PNGase F without any glycoprotein extraction. Released native glycans were purified and enriched by PGC-SPE. About 100 N-glycans were identified, profiled, and structurally elucidated by nano LC/MS and tandem MS. Sialylated N-glycans were exclusively present in abundance in live rat saliva while non-sialylated N-glycans including LacdiNAc disaccharides were detected in high level following death. Through in-depth investigations using quantitative comparison and statistical analysis, 14 N-glycans significantly changed after death were identified as the potential marker candidates for TSD estimation. This proof of concept study demonstrated the feasibility of saliva glycosylation for estimating time of death, with obvious forensic applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-203

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Near-infrared fluorescent probes for the detection of alkaline phosphatase activity in-vivo imaging

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Alkaline phosphatase (ALP) is a crucial biological enzyme for osteoblast activity during early osteoblast differentiation, but only few biologically compatible methods are available for its detection. Here, we developed highly selective, sensitive and fast responsive new near-infrared (NIR) fluorescence probes, NIR-Phos 1 and NIR-Phos 2, for the fluorescent detection of ALP. The NIR probes also displayed desired properties such as high stability and selectivity, showing a highly rapid “turn-on” fluorescence response rate completed within 1.5 min, on adding 0.1 U/mL ALP. By taking advantage of the superior properties of the NIR probes, we have demonstrated its utility in real-time monitoring of both the concentration- and time-dependent variations of endogenous ALP in living cells and animals, thereby providing a potentially powerful approach for probing ALP activity in biological systems.

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Code: **ANAL.P-204**

Area: Analytical Chemistry

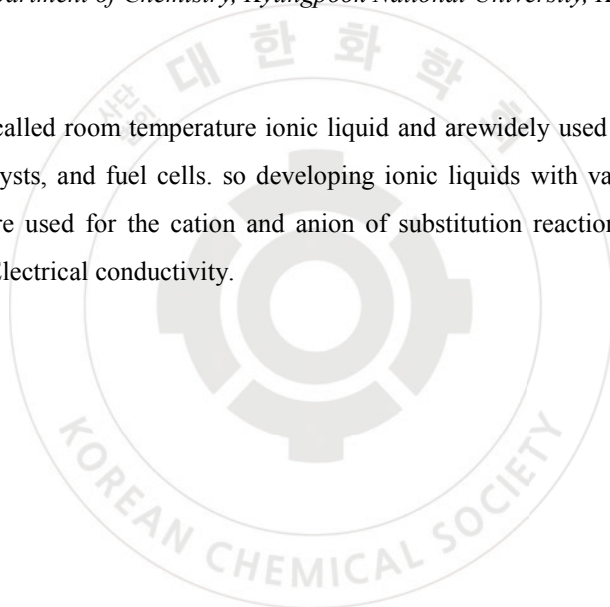
Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Alkaline Ionic Liquids for electrolytes of fuel cells

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these ionic liquids are called room temperature ionic liquid and are widely used in various fields besides organic synthesis, catalysts, and fuel cells. so developing ionic liquids with various properties in more easy way. solvents were used for the cation and anion of substitution reaction, and the synthesis was checked by IR, NMR, Electrical conductivity.



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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Contemporary Multispectral Three Dimensional Observation of Intracellular Organelles via Enhanced Dark-field Super-resolution Microscopy

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An innovative fluorescence-free super-localization approach for imaging intracellular organelles contacts at three dimension using dual-wavelength enhanced dark field microscopy (EDF). Mitochondria associated endoplasmic reticulum [mito-ER] was imaged by labelling the organelles with plasmon nanoparticles (NPs) of different scattering wavelength. The dual-wavelength synchronized EDF setup allows a concurrent imaging of both organelles under physiological conditions. The three dimensional super-localization of the NPs was achieved by fitting the center coordinates by least-cubic algorithm. The reconstructed super-resolution images resolved controversy over the distance between the intracellular organelles at functional contacts. The distance between the organelles was measured to be 45 nm, the distance fits to be the true feature of the organelles at functional contact site. The results designate to be the novel and reliable approach for the analysis of intracellular organelles at three dimension for accurate information under physiological conditions.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL.P-206

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

High Speed Spiral Scanning Spectrometry for reliable Quantitative Analysis of Ag/GO Nanocomposite SERS substrate

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Surface enhanced Raman spectroscopy (SERS) is a sensitive analytical tool in which weak Raman signal are enhanced by localized surface plasmon of noble metal nanoparticles or nanocomposites. In plural recent studies, analytical capability of SERS method, such as reproducibility and uniformity, has been examined with lithographic patterns, size controlled nanoparticles, and colloidal self-assembly. For quantitative SERS measurement, it is required to overcome the interference from the homogeneity substrates and the dispersity of analyte. In this study, we developed high-speed spiral scanning spectrometry for reliable quantitative analysis using flexible SERS substrate. It is a method of measuring whole analytes dispersed on a substrate by rotating and translating a 2-D cylindrical substrate. We measured crystal violet dye on flexible Ag/GO substrate using spiral scanning method. It showed a quantitative analysis curve, high sensitivity and ultra-uniformity. In addition, flexible SERS substrates can be applied to various analytical fields.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-207

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The electron transfer interaction between mediator and enzyme onto the electrode

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Multi-walled carbon nanotubes (MWCNTs) were modified with polydopamine (PDA) to composite the PDA@MWCNTs onto surface of MWCNTs for hydrophilicity. MWCNTs were homogeneously covered with a biocompatible PDA by a simple dip-coating approach in weak base solution. We prepared the PDA@MWCNTs using ultrasonication and stirring method in Tris-HCl buffer solution (pH 8.5). And the [Ruthenium(4,4'-dimethoxy-2,2'-bipyridine)₂Cl₂] ([Ru(dmo-bpy)₂Cl₂]) was synthesized by refluxing in ethanol to confirm the electron transfer effect with glucose oxidase (GOx). And then, we immobilized the [Ru(dmo-bpy)₂Cl₂] with GOx and poly(ethylene glycol) diglycidyl ether (PEGDGE) onto PDA@MWCNTs modified SPCEs. We investigated the electron transfer behaviors of our electrode using cyclic voltammetry (CV) amperometry. The results suggested that the efficiency of electron transfer between enzyme and mediator is important.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-208

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Simultaneous Detection of Thyroid Hormones based on Multi-Immuno- reaction by Dual-Wavelength Capillary Electrophoresis

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A novel dual-wavelength capillary electrophoresis (CE) technique with laser-induced fluorescence (LIF) detection has been investigated for the simultaneous separation and determination of thyroid stimulating hormone (TSH), thyroxine (T4), and triiodothyronine (T3). Thyroid hormones have been reported to influence various diseases such as thyroidectomy, thyroiditis, and hypothyroid. Thus, measurements of T4, T3, and TSH are helpful for the clinical evaluation of thyroid function. In this study, immuno-
reaction and biotin-streptavidin interaction were developed for highly sensitive detection of thyroid hormones as a function of separation efficiency and migration time. Various factors such as the pH of running buffer, separation voltage, and effective length were also examined in order to determine the optimum CE conditions. All three of standard thyroid hormones were analyzed within 3.2 min in 25 mM Na₂B₄O₇-NaOH buffer (pH 9.3) without losing resolving power under optimal conditions, which were 1,000-100,000 times more sensitive than other previous detection methods. Moreover, the CE with LIF detection method also successfully applied to the analysis of real human blood samples. As a result, the immuno-
reaction-based CE method with LIF detection is an effective, rapid analysis technique for highly sensitive detection of thyroid hormones related to thyroid gland disease.

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Code: ANAL.P-209

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ultra-sensitive Immunodetection of Cancer Antigen 125 based on Enhanced Plasmonic Scattering of Nano Probe by Dual-mode Wavelength-dependent Enhanced Dark-field Super-resolution Microscopy

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A ultra-sensitive immunodetection was achieved for the biomarker cancer antigen 125 (CA125), which was developed based on selected enhanced detection immunotag by dual-mode wavelength-dependent enhanced dark-field (EDF) microscopy. For simultaneous dual-detection, an color digital camera and electron multiplying cooled charge-coupled device camera were used for quantitative and qualitative analysis, respectively, based on the dark-field scattering images. To increase the efficacy of the scattering signal, various size of different plasmon nanoparticle (i.e., gold nanoparticles, 5 nm, 12 nm, 20 nm, 100 nm and 250 nm; silver nanoparticles, 20 nm, 30 nm, 40 nm, 80 nm and 100 nm) were used as the detection tags and investigated with wavelength dependence of the light source, and the quantum efficiency of the electron-multiplying charge-coupled device camera, 40-nm silver nanoparticle (SNP) was selected as an optimum fluorescence-free probe. CA125 was screened at single-molecule level and quantitatively analyzed by measuring the scattering signals of 40-nm SNP on gold-nanodots arraychip. CA125 was screened at single-molecule level and quantitatively analyzed with lowest possible possible LOD ($4 \text{ } \mu\text{g/mL}$, S/N = 3) and a wide dynamic detection range of $4 \text{ } \mu\text{g/mL}$ -80 U/mL ($R = 0.9935$), which was a over the 100 times lower LOD and wider dynamic range than previous researches. Dual-mode EDF based optical property of the plasmon scattering signal of metal nanoparticles allowed us for a of disease related biomolecules at single-molecule level for early diagnosis of life threatening diseases.

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Code: ANAL.P-210

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Size-based fractionation and characterization of starch granules using split flow thin cell (SPLITT) and gravitational field-flow fractionation (GrFFF)

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Starch is obtained from cereals (corn, potato and rice), and is used in food, paper, mining industries, and in the production of adhesives. Starch granules from various botanical sources vary widely in the granular size and shape as well as in the composition of amylose, amylopectin and protein, thus leading to differences in functional properties and industrial applicability. In addition, size of starch granules has an important influence on the enzymatic reaction. The sieving may be used for size-based fractionation of granules. However it may induce damage of starch granules by mechanical force. The split flow thin cell (SPLITT) is a separation technique that provides fractionation of a polydispersed sample into two size fractions. SPLITT uses an open channel, and thus mechanical damages could be minimized. It can also be used in a large scale as the sample can be fed continuously. In this study, SPLITT was employed for a size-based fractionation of various starch granules (corn, potato) in a large scale. The SPLITT fractionation results were checked by optical microscope (OM) and gravitational field-flow fractionation (GrFFF). Then the size-fractions of the starch granules were analyzed by differential scanning calorimetry (DSC). Results from DSC suggested that the composition of the starch granules may vary with their sizes and types.

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Code: ANAL.P-211

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Variation of separation efficiency of glycogen and pullulan with channel type in field-flow fractionation (FFF)

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Field-flow fractionation (FFF) is a family of tools for the separation and characterization of particles and polymers. It has a broad dynamic range, and the utilization of an open channel requires no packing material, minimizing problems of sample adsorption, degradation and loss than in size exclusion chromatography (SEC). Frit inlet asymmetrical flow field-flow fractionation (FI-AsFIFFF) is a modified form of the asymmetrical field-flow fractionation (AsFIFFF) technique. Relatively higher carrier flow through the frit relative to the sample injection flow compresses the incoming sample band toward the accumulation wall of the channel. The main advantage of FI-AsFIFFF is to bypass the focusing step for relaxation in FIFFF that are normally carried out by stopping the carrier flow for a period of time to establish an equilibrium condition of the sample components. In this study, the separation efficiencies such as resolution, plate height and recovery were compared between AsFIFFF and FI-AsFIFFF channel using glycogen and pullulan. It was found that FI-AsFIFFF yields higher sample recovery than AsFIFFF. However, the resolution of FI-AsFIFFF was lower than that of AsFIFFF (about half). The resolution was increased with increasing the cross flow rate in both channels. Results also indicated that the resolution, plate height and the sample recovery changes with the type of samples. It seems a care needs to be taken in choosing the channel type in FFF studies.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL.P-212

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Effect of light on size of *chlorella sorokiniana* and production of glutathione using gravitational field-flow fractionation (GrFFF)

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chlorella sorokiniana (or simply, *chlorella*) is one of single-cell green microalgae and has the size range of 2~10 μm . It plays an important role in food as it provides a rich source of carbohydrates, vitamins and proteins. It can also produce the glutathione, which is one of important antioxidant in plants, animals, fungi and some bacteria. The antioxidant-production capacity of the *chlorella sorokiniana* is determined by various parameters including pH, temperature, and the presence of light. Previous studies have been mainly focused on the application of the *chlorella*, and basic studies on the relationship between the antioxidant-production capacity of the *chlorella sorokiniana* and these parameters are insufficient. In this work, the change in the size of the *chlorella sorokiniana* with the presence of light was studied, and then the effects of the size, the presence of light, and incubation time on the capacity of the *chlorella sorokiniana* for production of glutathione were investigated. The size of *chlorella sorokiniana* was determined using an optical microscopy (OM) and gravitational field-flow fractionation (GrFFF). GrFFF is a gentle elution-based separation technique that is known to be useful for separation of micron-sized particles. The glutathione produced from *chlorella* was analyzed quantitatively using a UV/Vis spectrophotometry. Both the size and number of *chlorella sorokiniana* were increased with increasing incubation time until 96 hours, and then were remained constant. The concentration of glutathione also was increased with the incubation time until 96 hours, after which was decreased.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Identification of behavior of synthesized Sm₂O₃ particles in goldfish

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Rare-earth nanoparticles are generally harmless in the environment, and could be utilized as a tracer for circulation process of nature. The rare-earth nanoparticles can be identified (or analyzed) by gamma ray irradiation, as they are decomposed by the gamma ray irradiation to yield radioactive rare-earth isotopes, producing their own characteristic signals. Gamma-ray irradiation is known to be highly sensitive for analysis of samples of trace concentrations. In this study, samarium oxide (Sm₂O₃) nanoparticles were synthesized by a sono-chemical method, and were analyzed using various techniques including asymmetrical flow field-flow fractionation (AsFIFFF), dynamic light scattering (DLS), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD) and inductively coupled plasma-mass spectroscopy (ICP-MS). AsFIFFF and DLS were used to determine the size distributions of the Sm₂O₃ particles. EDX and XRD were used to determine the chemical composition of nanoparticles. The presence of samarium was confirmed by the XRD and EDX results. The AsFIFFF and DLS results showed the Sm₂O₃ nanoparticles have sizes ranging about 20 ~ 30 nm. The Sm₂O₃ nanoparticles were fed to gold fish, then the concentration of the particles in various organs of the gold fish were analyzed using ICP-MS.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ANAL.P-214

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Optimization of liquid chromatography mass spectrometry (LC/MS) for the analysis of the ganglioside isomers

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Gangliosides are acidic glycosphingolipids which contain sugar chains with a variety of sialic acid residues. There are hundreds of variations in ganglioside structures based on compositions and structures of oligosaccharide head groups as well as compositions of ceramide cores. However, most LC/MS studies did not include separation of these structural isomers. Therefore, we tried to optimize LC conditions for resolving ganglioside isomers and we specifically focused on developing separation conditions for resolving structural isomers of disialogangliosides, designated to GD1a and GD1b, which are known to be major species in mammal brains. Through optimization processes, we developed an effective LC condition with a conventional C18 column and an appropriate salt additive. And we applied the optimized LC/MS method to the analysis of the total ganglioside extract from porcine brain and successfully analyzed individual isomers of di- and tri- gangliosides.

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Code: ANAL.P-215

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Investigation of sample preparation and analysis methods for profiling organic chemicals and metals in teeth

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Recently, due to its specific structure and growth pattern, deciduous teeth have been proposed to be retrospective temporal biomarkers for exposomics researches which try to assess comprehensively environmental exposures from the fetal period onwards. However, sample preparation and analysis steps for teeth samples have not been explored extensively and need to be standardized. In this study, we investigated various sample preparation procedures and mass spectrometric methods for profiling organics and metals present in teeth samples. In order to evaluate sample preparation procedures including sampling, pulverization, incubation, and extraction, we employed paper spray ionization (PSI) mass spectrometry (MS), paper cone spray ionization (PCSI) MS, and MALDI MS. In addition, we tested various LC/MS methods for organic chemical analysis and laser ablation-based elemental mapping methods for spatially resolved metal analysis.

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Code: ANAL.P-216

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The structural characterization of disease related human transmembrane proteins using the NMR spectroscopy

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Human transmembrane proteins (hTMPs) play essential roles in cellular metabolism, participating in processes such as ion transport, nutrient uptake, signal transduction, and intercellular communication. However, aggregation or misfolding of hTMPs due to unwanted mutations of amino acid sequences or errors in the folding process leads to an increase in various human diseases. Therefore, we aim to create new treatments that can inhibit or eliminate these changes. In this research, we tried to identify the structure of human amyloid- β (hA β) and human melanocortin-4 receptor (hMC4R). The hA β transmembrane protein shows that the non-fibrillar hA β s form the Ca²⁺-permeable ion channel in the cell membrane and these channels can disrupt the normal cellular calcium homeostasis. It plays an important role in pathogenesis of dementia and Alzheimer disease. The human melanocortin-4 receptor (hMC4R) has been highlighted because it is central regulator of body weight. Heterozygous mutations related in genetic cause of severe obesity. We succeed to produce the transmembrane domain of the hA β and second transmembrane domain of the wild-type hMC4R and mutant hMC4R. In cases of the wt/m-TM2 purification, we used sodium dodecyl sulfate (SDS) because of their hydrophobicity. Since SDS binds so strongly to protein, it interferes with biophysical techniques used for characterization of wt/m TM2. Thus, we developed the removal methods of SDS to obtain high quality of purification for wt/m-TM2. Highly purified proteins were applied to several analysis techniques like PAGE, CD, MASS, solution and solid-state NMR spectroscopy. In addition, we could get ¹H-¹⁵N 1D, 2D SAMMY and SAMPI spectra using home-built solid-state NMR probe.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Diverse home-built solid-state NMR probes for specific purposes

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The solid-state NMR has been used to investigate insoluble materials in advanced industrial site. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. We will 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 narrow-bore(NB) ^1H - ^{15}N solid-state NMR probe for these electrically lossy samples. Li-ion battery and LCD panel have been grown up rapidly as a front-runner in technology-intensive industry. Their microstructural changes are the reason of battery efficiency drop and defective pixel. We will also present a home-built 500 MHz NB ^{19}F - ^{13}C solid-state NMR probe with flat-square coil for analyzing LCD panel and 600 MHz NB ^{19}F - ^7Li solid-state NMR probe 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 batterypack samples. These two probes provide high efficiency and good RF homogeneity. And finally we will introduce our recent commission task project "Development of sample dependent Solid- state NMR probe for the analysis of nanomaterials". The ^{19}F - ^{13}C solid-state 400 MHz NB probe was made and quality test was in progress.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ANAL.P-218

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development for simultaneous purification of nerve agent metabolites using MB-Ab complex and affinity gel and application to nerve agent inhibited rhesus monkey plasma

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A sensitive method for the purification and determination of two protein adducts, organophosphorus (OP)-BuChE and OP-albumin adducts, in a single sample using a simultaneous sample preparation method was developed and validated using liquid chromatography-tandem mass spectrometry (LC-MS/MS). First, we isolated O-ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (VX) and O-pinacolyl methylphosphonofluoridate (soman, GD)-BuChE adducts using an immunomagnetic separation (IMS) method and the HiTrap Blue affinity column was subsequently used to isolate and purify VX and GD-albumin adducts from the plasma of rhesus monkeys exposed to nerve agents. Additionally, we examined the time-concentration profiles of two biomarkers, VX and GD-nonapeptide and VX and GD-tyrosines, derived from OP-BuChE and OP-albumin adducts up to 8 weeks after exposure. Based on the results, we determined that VX and GD-tyrosine is more suitable than VX and GD-nonapeptide as a biomarker owing to its longevity. This integrated approach is expected to be applicable for the quantification of other OP-BuChE and OP-albumin adducts in human plasma, thus serving as a potential generic assay for exposure to nerve agents. Keywords: immunomagnetic separation; chemical warfare agent; butyrylcholinesterase; albumin; UPLC-MS/MS

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Code: **ANAL.P-219**

Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Optimization of Preparation Condition for Analysis of Statins and Fibrates Adulterated in Oil type Dietary Supplements

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The incidence of hyperlipidemia, which is one of cardiovascular diseases, has increased due to changes in westernized dietary habits of modern humans. Fibrate derivatives and statins which are HMG-CoA reductase inhibitors are representative drug components for treating hyperlipemia. However, these medicines may cause various side effects due to long-term dose. For this reason, consumers purchase dietary supplements such as form of oil soft capsules containing natural omega-3 fatty acids. Sometimes, there are cases in which unauthorized components is added to improve their pharmacological efficacies. Thus, it is necessary to investigate the illegally adulterated components in dietary supplements using the optimized preparation and analytical methods. In this study, to find out the optimum preparation condition for oil soft capsules, normal hexane (A) and 70% MeOH (B) mixture were selected as liquid-liquid extraction (LLE) solvents. The ratios of A and B were changed as follows; 3:1, 2:1, 1:1, 1:2, and 1:3 (v/v), respectively. After preparation, all samples were analysed by ultra performance liquid chromatography (UPLC), in triplicate. In conclusion, only the recovery of 1:1 ratio was confirmed at 80 ~ 120%. Therefore, a suitable ratio of the LLE solution for detecting the statins and fibrates adulterated in oil type dietary supplements is 1:1, and it is considered that can be used as a more effective preparation condition.

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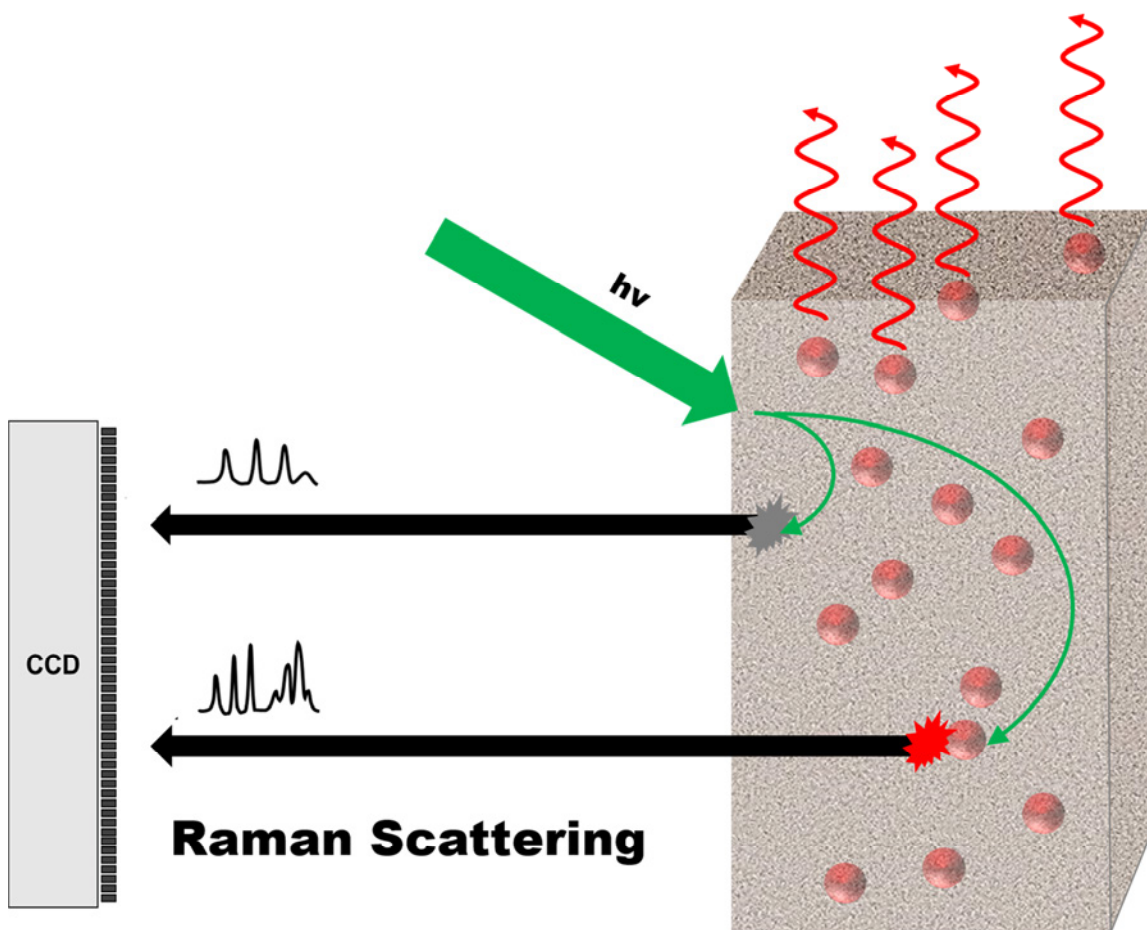
Type: Poster Presentation, Time: THU 11:00~12:30

Wide-depth Spatially offset Raman Spectroscopy for Detecting Hazardous Chemicals in Building Materials

Youngho Cho, Chan Ryang Park, Hyung Min Kim^{*}

Department of Chemistry, Kookmin University, Korea

Toxic chemicals inside building materials must be detected early to prevent secondary damage because the chemical have long-term harmful effect on the human body. Although deep Raman spectroscopy is a potential candidate for inside harmful materials detection, it is very difficult to distinguish the Raman signal of the inside chemicals from the background signal of surrounding building materials. In this study, we developed wide-depth spatially offset Raman spectroscopy (W-SORS) coupled with a processing algorithm to identify inside chemicals. Furthermore, we proposed a method of measuring the thickness of an external building materials through signal processing of the W-SORS spectral slope.



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Fast Direct Apolipoprotein E Genotyping for Alzheimer's by Multi-channel Microchip Electrophoresis

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A direct apolipoprotein E (apoE) genotyping-based multi-channel microchip electrophoresis (ME) method was developed for fast high-throughput screening of Alzheimer. The target apoE polymorphism genes (i.e., 112 bp, 253 bp, 308 bp, 444 bp, and 514 bp DNA) were amplified by only 10 cycles of one-step multiplex polymerase chain reaction (PCR) from whole blood without DNA extraction. The amplified target DNA fragments were detected in 20 s by a programmed electric field strength (PEFS)-based single-channel ME. According to the optimum conditions of single-channel ME, target DNA fragments were separated using various multi-channel ME with three and five parallel channels, which simultaneously detected within 20 s without any loss of resolving power or reproducibility. The proposed multi-channel ME-PEFS assay technique provides a simple and accurate method for fast high-throughput screening of Alzheimer's disease, which can be simply apply to more large number of parallel channels for more high-throughput screening.

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Type: Poster Presentation, Time: THU 11:00~12:30

Identification of Diverse Types of Monosaccharide Derivative Isomers By Host-guest Complexation with Cucurbit[7]uril

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Distinguishing constituent monosaccharides in target carbohydrate using mass spectrometry (MS) remains challenging due to their undistinguishable fragmentation patterns induced by their isomeric structures and similar physical properties. Although a carbohydrate is composed of diverse monosaccharide/monosaccharide derivative species, previous methods focused on one or two types of monosaccharides and monosaccharide derivatives. Therefore, it is necessary to invent a novel approach to be developed as a comprehensive method for identification of diverse types of monosaccharides and monosaccharide derivatives. Our study reveals that the combination between host-guest and gas-phase chemistry is effective for identifying diverse types of monosaccharide derivative isomers. Four different types of monosaccharide derivative isomers were investigated herein as target monosaccharide derivative species. A host molecule, cucurbit[7]uril (CB[7]), was utilized herein due to its high recognition ability in monosaccharides. It was observed that each monosaccharide derivative forms gas-phase complex with CB[7] while most of bindings between the CB[7] and target guests are negligible in aqueous solution. Tandem MS study shows that the monosaccharide derivatives have different fragmentation patterns in their complexes with CB[7], allowing their identification. Structural studies using ion mobility MS and computational calculations suggest that the slight structural differences between the isomers are augmented by their distinct host-guest interactions with CB[7] in the gas-phase. Overall, the present study reveals that our gas-phase host-guest system can be developed as a comprehensive method for qualitative analysis of constituent monosaccharides in target carbohydrates.

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Simultaneous determination of 21 tar colors in lipsticks by ultra-performance liquid chromatography

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A rapid and precise analytical method of 21 tar colors was developed for identification of coloring constituents in lipsticks using ultra-performance liquid chromatography (UPLC). The 15 water-soluble and 6 water-insoluble tar colors were extracted by 20% methanol and chloroform, respectively. And then chloroform extracted solution applied solid-phase extraction (SPE) method for clean-up. The chromatographic separation was achieved on ACQUITY UPLC BEH C18 (2.1 mm × 100 mm, 1.7 μm), the gradient LC method employs solutions A and B as mobile phase. The solution A contains 10 mM ammonium formate in distilled water and solution B contains acetonitrile/methanol(1:1). The method was validated for specificity, linearity, limit of detection, limit of quantification and recovery. The linear relationships of the 21 colorant compounds were demonstrated with R^2 values higher than 0.995. The recoveries ranged from 83.9% to 105.3 % with the relative standard deviations (RSDs) less than 7 % (n=3).

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Potential biomarkers of diabetic kidney disease detected by NMR-based metabolite profiling

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Previous studies described metabolite profiles of diabetic animals; however, they were highly variable because of heterogeneity of the studies. We aimed to characterize the metabolite changes in the early and late stages of diabetic kidney disease to suggest potential biomarkers for early detection and its progression. Metabolite profiling using high-resolution nuclear magnetic resonance spectroscopy and multivariate statistical analysis was performed in *db/db* mice. We compared concentrations of serum and urinary metabolites between *db/m* and *db/db* mice at 8 or 20 weeks of age and investigated whether changes between 8 and 20 weeks in each group were significant. Correlation analysis was used to determine associations between urinary metabolites and urinary albumin excretion. Partial least squares-discriminant analysis score plots showed a significant distinction between *db/m* and *db/db* mice. The metabolic profiles demonstrated significantly increased urine levels of glucose and tricarboxylic acid cycle intermediates, such as fumarate, citrate, and 2-oxoglutarate, at both 8 and 20 weeks in *db/db* mice. These intermediates also exhibited strong positive associations with urinary albumin excretion, suggesting that they may be potential biomarkers for early diagnosis. On the contrary, branched chain amino acid and homocysteine-methionine metabolism were activated early in the disease, whereas ketone and fatty acid metabolism were significantly changed in the late phase of the disease. We demonstrated phase-specific alterations in metabolites during progression of diabetic kidney disease. This study provides insights into perturbed mechanisms during evolution of the disease and identifies potential novel biomarkers for diabetic kidney disease.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly sensitive detection of lethal infectious pathogen using SERS-based lateral flow assay

Rui Wang, Kihyun Kim, JAEBUM CHOO*

Department of Bionano Technology, Hanyang University, Korea

Effective identification of pathogenic bacteria is important for biodefense. In recent years, microbiological culture and colony counting, polymerase chain reaction (PCR) or immunoassay has been considered as a gold standard for the detection of pathogens including toxin, bacteria and virus. However, these methods cannot meet the requirement of rapid and highly sensitive detection because they need long sample preparation time and have limited detection sensitivity. Therefore, it is still urgent to develop a new method for the rapid and sensitive detection of pathogens for preparedness of bioterrorism. In this presentation, we introduce a new pathogen assay technique using a surface-enhanced Raman scattering (SERS)-based lateral flow assay. Two different antigens, including botulinum toxin A and *Yersinia pestis* have been selected as detection targets. According to our assay results, the limit of detection of botulinum toxin A and *Yersinia pestis* using the SERS-based lateral flow platform was 10 pg/mL and 102 CFU/mL, respectively, which are three orders of magnitude more sensitive than that of commercial rapid kit. Thus, the proposed SERS-based lateral flow assay has a strong potential to be a valuable tool in the early detection of a specific pathogen due to its excellent analytical sensitivity.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Rapid and sensitive detection of highly risk pathogens using SERS-based lateral flow assay

Kihyun Kim, Rui Wang, JAEBUM CHOO*

Department of Bionano Technology, Hanyang University, Korea

Bioterrorism has been received great concerns after the 2001 anthrax attacks in United States. Highly risk pathogens used in the bioterror are greatly contagious and also have a high fatality. To minimize life damages from bioterror, rapid and sensitive detection methods of specific pathogen is urgently required. To date, various detection methods including direct counting of bacteria, polymerase chain reaction (PCR), and immunoassay have been developed but they do not satisfy the requirements in the field due to complicated sample pre-treatment procedures, long detection time and low sensitivity. To resolve those problems, we recently developed a SERS-based detection technique for the detection of various pathogens. In this poster, we introduce a new pathogen assay method using a SERS-based lateral flow assay. Two different pathogens, *Bacillus anthracis* and *Francisella tularensis* have been selected as detection targets. In the case of *Francisella tularensis*, the limit of detection measured by the SERS-based lateral flow platform was estimated to be 10^2 CFU/mL, which is three orders of magnitude more sensitive than that of commercial ELISA kit. Therefore, the proposed SERS-based lateral flow assay technique has a strong potential to be used as a valuable tool in the early detection of a specific pathogen due to its simplicity and excellent analytical sensitivity.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Application of gradient generating microdroplet-based chips for rapid and sensitive bioanalysis

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Department of Bionano Technology, Hanyang University, Korea

Microfluidic technology have recently emerged as an efficient tool for the study of various chemical or biological reactions. Recently, we reported that high-throughput chemical or biological reactions could be performed in a continuous flow microfluidic channel with an automatic manner. However, there is a “memory effect” problem in the continuous flow system. Samples in the continuous stream could be stacked in the wall of a microfluidic channel, and they may occur unwanted flow hindrance. To resolve this problem, we recently developed a novel gradient microdroplet system. In this system, the sample stacking problem can be solved since two-phase liquid/liquid segmented flow reduces the memory effect. A serial dilution of reagent can be achieved in a stepwise manner using microfluidic concentration gradient generators. Then, desired concentrations of a reagent were 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 effects for various concentrations of a reagent.

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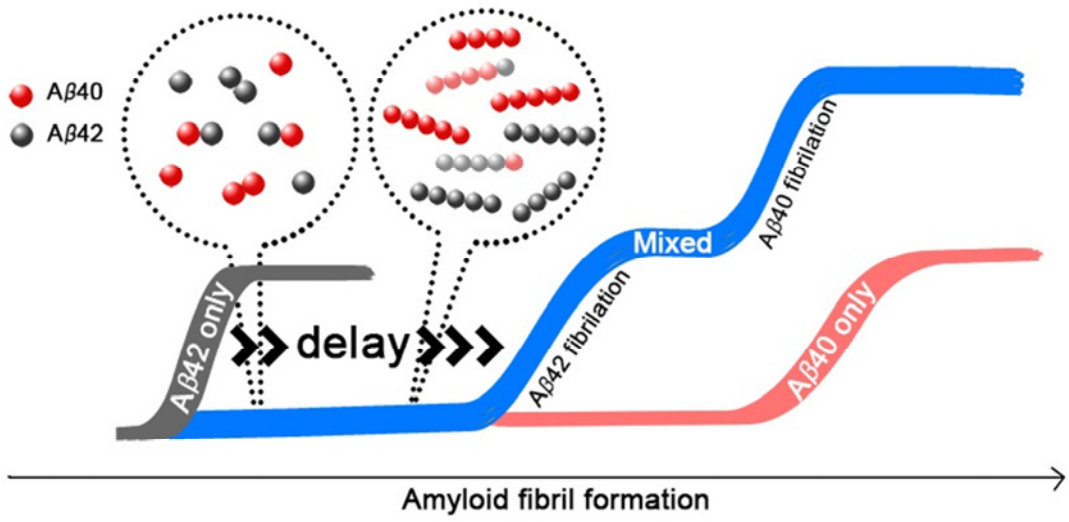
Type: Poster Presentation, Time: THU 11:00~12:30

Investigation of the homo- and hetero-oligomerization of amyloid- β 1-40 and 1-42 using electrospray ionization mass spectrometry

Chae Eun Heo, Taesu Choi^{*}, Hugh Inkon Kim^{*}

Department of Chemistry, Korea University, Korea

Self-assembly of amyloid- β peptides ($A\beta$) has accepted as an important issue, because the final product of the self-assembly (i.e. amyloid fibrils) is highly relevant to the Alzheimer's disease (AD). Among various $A\beta$ alloforms, $A\beta$ 1-42 ($A\beta_{42}$) and $A\beta$ 1-40 ($A\beta_{40}$) are mainly involved in $A\beta$ fibril formation. The self-assembly mechanisms of $A\beta_{42}$ and $A\beta_{40}$ are known to be different and $A\beta_{42}$ and $A\beta_{40}$ can form hetero-assemblies through their cross-interaction. However, the role of hetero-assemblies of a mixture of $A\beta_{42}$ and $A\beta_{40}$ is not yet fully understood. Thus, characterizing the cross-interaction between $A\beta_{42}$ and $A\beta_{40}$ is crucial for understanding the role of hetero-assemblies during the fibrillation of mixed $A\beta$ peptides. In this research, we demonstrated the influence of the cross-interaction of $A\beta_{42}$ and $A\beta_{40}$ in the early stage of fibrillation. We monitored the fibrillation process of $A\beta_{42}$, $A\beta_{40}$ and their 1:1 mixtures using thioflavin T (ThT) assay and electrospray ionization mass spectrometry (ESI-MS). Then, we further investigated the preference for homo- and hetero- oligomerization of $A\beta_{40}$ and $A\beta_{42}$ using ion mobility spectrometry (IMS) along with solution small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations. Our results suggest that the competitive self-assembly of $A\beta_{42}$ and $A\beta_{40}$ plays a pivotal role in disturbing homo-oligomerization of $A\beta_{42}$ in the early stage of fibrillation.



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Developed to Overhauser Dynamic Nuclear Polarization Nuclear Magnetic Resonance Systems for Signal Enhancement

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Nuclear magnetic resonance (NMR) spectroscopy has advantages such as non-destructive observation of molecular structure and dynamics, analysis of amorphous samples, and high selectivity of nuclear species to be observed. However, NMR has the disadvantage of low sensitivity because it uses low energy. In order to overcome the disadvantage of NMR, overhauser dynamic nuclear polarization (ODNP) NMR system which amplifies NMR signals from several tens to several hundred times using the interaction of electron spins and nuclear spins within about 1 nm from the electron spin centers. Therefore, a local region can be designated by selectively positioning the spin markers in the sample. ODNP NMR can be used to measure the diffusion rate of water in a variety of materials and to measure the dependence of binding between protein and water on solvents. In our laboratory, an Electron Paramagnetic Resonance (EPR) spectrometer and NMR components (radio frequency pulse modules, NMR tuning boxes, ODNP NMR probes, etc.) has been assembled together and instrumental optimization for the best amplification is currently in progress.

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A Method for Quantitative Analysis of Cellular Uptake in Combination Therapy Treating Neuroblastoma

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Neuroblastoma is fourth most abundant malignant tumor in childhood which begins when immature nerve cells grow out of control. As Neuroblastoma belongs to heterogeneous disease, chemotherapy has been underway as combination of various anticancer drugs. Therefore, to optimize combination chemotherapy for diverse case, understanding how combination therapy works better than single drug is crucial. However, relevant researches so far have been focused on only combination efficiency in clinical investigation. In this research, we aim to study cellular uptake of combination therapy in correlation to drug efficiency for cancer cells, compared to single drug regimen. Firstly, cell viability test for neuroblastoma cell lines, SK-N-SH and SH-SY5Y, was conducted using each drug in combination therapy to search proper drug treating condition. Also, we tried to develop quantitation method based on mass spectrometry for drug in cell culture media. As a result, we optimized solvent condition for maximizing drug ionization efficiency in mass spectrometry and pretreatment method of culture media to quantify small molecules such as drugs. With aforementioned results, we are currently working on the correlation between treatment efficiency and time-based cellular uptake after using combination or single drug.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Metabolic profiling in heart tissue of mice fed atherogenic diet

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¹*Korea Basic Science Institute, Korea*

Atherosclerosis is a leading cause of cardiovascular disease characterized by thickening of the arterial wall resulting from abnormal lipid accumulation. In atherosclerosis model, most of the studies illustrated the mechanism of atherosclerosis in biofluids and/or liver but not in heart. In the present study, we performed metabolic profile in heart tissue during the progression of diet-induced atherosclerosis mouse model using liquid chromatography/mass spectrometry (LC/MS). A lipidomics approach was used to investigate the changes in lipid species in heart tissue from AD mice. Principal component analysis (PCA) plots showed a clear differentiation between normal diet (ND) and atherogenic diet (AD) groups in both positive and negative ion modes. In the PCA score plots, significant discriminations between ND and AD groups was observed in each time point (8 weeks, 16 weeks, and 25 weeks). Cers were significantly decreased in AD group, whereas GlcCers were increased in AD group. Saturated fatty acids including FFA 16:0 (palmitic acid) and FFA 18:0 (stearic acid) were significantly increased in AD, whereas unsaturated fatty acids were decreased. TG species were changed depending on the length of acyl chain and degree of unsaturation. Also we assessed quantitative analysis of suffer-containing amino acid (SAA) metabolites which is related with stearyl-CoA desaturase-1 (SCD1) because SCD1 produces monounsaturated fatty acids from saturated fatty acids. The levels of SAA metabolites in heart tissue were significantly changed in AD mice. This study demonstrates that LC/ MS based metabolic profiling can be used to understand metabolism in heart tissue of diet-induced atherosclerosis animal model and may provide the insight for molecular aspects of cardiovascular diseases.

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Facile Fabrication of Nanostructured Surfaces Amenable to Laser Desorption/Ionization of Drug Molecules

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Herein, we present a facile strategy to bring the LDI (laser desorption/ionization) capability onto nanostructured surfaces, which can further be tailored with various surface coatings suitable to individual applications. While the MALDI (matrix-assisted laser desorption/ionization) method has been a powerful tool to ionize thermally labile molecules such as biological and synthetic polymers, the intrinsic use of excess matrixes causes certain limitations on its applications. To overcome the related issues, matrix-free LDI methods have been demonstrated in recent years; in particular, a variety of nanostructures were exhibited for their LDI capability, most of which are unfortunately too special to be prepared by other laboratories. In this presentation, we present a simple and facile strategy of how to get certain surface nanostructures to achieve the LDI capability by using known techniques of surface chemistry. The strategy is based on the thermal mechanism that would promote intact desorption of thermally labile molecules by laser-induced surface heating. The produced LDI nanostructured surfaces can further be decorated by surface coatings to possess the suitable surface properties for individual applications, such as hydrophobic, hydrophilic, and non-fouling properties. All these can be done by simple and known chemistry. In addition, this strategy is applicable to virtually any nanostructured surfaces. In this work, the strategy is demonstrated on conical AAO (anodized aluminum oxide) templates with respect to LDI of drug molecules with moderate molecular weights of 500 to 1000 Da.

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Metabolomic analysis of polychlorinated biphenyls(PCBs) and organochlorine pesticides(OCPs) exposure in human plasma

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Polychlorinated biphenyls(PCBs) and organochlorine pesticides(OCPs) are types of persistent organic pollutants (POPs) known as lipophilic environmental toxins. Accumulation of POPs has adverse effects on both environment and human. However, few studies have assessed their internal exposure to POPs. The objective of this study was to observe the effect by accumulation of POPs in humans and to investigate the associations between POPs levels and metabolic profiles in plasma samples. In this study, concentrations of total 33 POPs including 16 PCBs and 17 OCPs were analyzed from plasma samples of 300 Koreans without occupational exposure to POPs. The sum of the signed ranks of five PCBs and six OCPs, respectively, were used in multivariate regression tools adjusted for age, sex, BMI, education, smoking and alcohol intake. Then, we performed plasma metabolic profiling using ¹H-NMR spectroscopy. We found that PCBs were significantly associated correlated with creatine, glucose, mannose, citrate, and phenylalanine. On the other hands, OCPs were correlated with creatine, mannose, lactate, and phenylalanine. This study suggests that the NMR-based metabolomic approach may provide a promising technique to understand the alteration of human metabolism and to identify potential biomarkers for estimating exposure effect of environmental toxins like POPs.

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Structure Elucidation and Potential Function study of Microcystin-LR

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The microcystin is a cyclic heptapeptide from metabolites of cyanobacteria in the genera *microcystis*, *anabaeba* as a result of eutrophication. It has been known that microcystin-LR is a potent inhibitor of the catalytic subunits of protein phosphatase-1(PP-1) as well as powerful tumor promoter. The active site of microcystin actually has two metal ions Fe^{2+}/Zn^{2+} close to the nucleophilic portion of PP-1-microcystin complex.

We report the isolation and purification of this microcystin-LR from cyanobacteria (blue-green algae) obtained from Daechung Dam in Chung-cheong Do, Korea. Microcystin-LR was extracted from solid-phase extraction (SPE) sample preparation using a CN cartridge. The cyan bacteria extract was purified to obtain microcystin-LR by HPLC method and identified by LC/MS. The solution structure of this compound was investigated with ¹H-NMR and 2D NOESY experiments were accomplished in DMSO-d₆ and signal assignment of microcystin-LR. On the basis of these distance data, distance geometry and molecular dynamic were carried out to determine the tertiary structure of microcystin-LR.

The detail structural studies that can elucidate the possible role of monovalent and divalent metal ions in PP-1-microcystin complication were carried out by utilizing molecular dynamics. Conformational changes in metal binding for ligands were monitored by molecular dynamic computation and potential of mean force (PMF) using the method of the free energy perturbation. The microcystin-metal binding PMF simulation results exhibit that microcystin can have very stable binding free energy of -10.95 kcal/mol by adopting the Mg^{2+} ion at broad geometrical distribution of 0.5~4.5 Å, and show that the K^+ ion can form a stable metal complex rather than other monovalent alkali metal ions

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Multimodal analysis of Polymer Blending (ABS/Nylon6) during Reliability Test: Mechanical and chemical analysis

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Blends of nylon 6 with acrylonitrile–butadiene–styrene (ABS) materials were prepared and investigated over a change of composition and mechanical strength during the reliability test under high temperature and humidity condition (50°C/90%RH ~ 4 weeks). The morphological change of the injection molded specimens were also observed before and after reliability test by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The change of mechanical properties were also investigated from micro to nanoscales during the reliability test; tensile strength measurement by universal testing machine and nanometer force measurement by atomic force microscopy. Under the reliability condition after 1 week, tensile strength of the sample were reduced by around 20% and the same trend of nanometer force changes were observed at the mapping image by AFM. The bulk and surface chemistry under the condition were also compared to understand the chemical degradation. Poly dispersity Index (PID) by gel permeation chromatography decreased by around 6% while surface chemistry by FTIR were not much changed. Herein, we present the degradation of the polymer blending during the reliability test using multi scale analytical tools.

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Area: Analytical Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Feasibility of 3-Phase direct immersion in-tube microextraction comparison with Single drop microextraction coupled with capillary electrophoresis

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Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME using commercial kits, LPME usually require more manual maneuvers. To overcome such shortcomings of LPME, we developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease using a commercial CE instrument. Here, we demonstrate direct immersion (DI)-ITME in a 3-phase configuration to enrich acidic compounds from an acidified aqueous sample to a basic acceptor plug through a thin organic phase. The feasibility and drawback of DI-ITME were investigated in comparison with direct immersion single drop microextraction (DI-SDME). Due to the lack of a hanging drop used in DI-SDME, DI-ITME is a quite simple and robust extraction method.

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Investigation on The Stability of Uric Acid and Its Isotope (1,3-15N2) in Ammonium Hydroxide for The Absolute Quantification of Uric Acid in Human Serum

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In clinical diagnosis, it's well known that the abnormal level of uric acid (UA) in human body is implicated in diverse human diseases, for instance, chronic heart failure, gouty arthritis, diabetes, chronic renal failure, and kidney stones). In order to accurately diagnose UA-related diseases, the development of the method for the absolute quantification of UA in biological sample is required. As a primary method, an isotope dilution mass spectrometry (IDMS) has been used to obtain the accurate quantity of UA in blood or serum and also develop the certificated reference material (CRM) so as to provide a SI-traceability to clinical laboratories. Due to the low solubility of UA in water, an ammonium hydroxide (NH₄OH) has been considered as a promising solvent to increase the solubility of UA and prepare both UA and its isotope standard solution for next IDMS-based absolute quantification. But, because of using this NH₄OH solvent, it gives rise to the unwanted degradation of UA. In this study, we sought to optimize condition for the stability of UA in NH₄OH solution by varying the mole ratios of UA to NH₄OH at five different mole ratios of 1/1, 1/1.5, 1/2, 1/3, and 1/5.6, followed by LC-ID-MRM analysis. In addition, we also inspected minutely the effect of the storage temperatures [-20 °C and room temperature (RT)]. Finally, we performed the quantitative analysis of UA containing the KRISS serum certificated reference material (CRM, 111-01-02A) with diverse mixing ratios of UA to NH₄OH and then compared those values to its certification value.

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Classification of glycoproteins by pattern identification in traditional Korean medicine (TKM) in human plasma from lung cancer patients

Jihoon Shin, jinwook lee, Min-gyu youn, miseon jeong, Jeonghoon Kang, Wonryeon Cho *

Department of Bio-nanochemistry, Wonkwang University, Korea

Patients have difficulties in seeking treatments based on Traditional Korean Medicine (TKM) because of the lack of standardized diagnosis. This study is a preliminary research for patient-specific TKM aiming at the discovery of biomarker for lung cancer diagnosis using the proteomics approach. Glycoproteins are well-known to be associated with diseases (especially cancers) and can be used as biomarkers for corresponding diseases. Six groups (EX, ES, EN, RX, RS and RN) from Lung cancer patients are independently analyzed through glycoproteomics approach based on the pattern identification in TKM. This lead to (1) establish the standardized methodology with proteomics for the pattern identification of lung cancers under the framework of TKM; (2) discover lung cancer biomarkers using TKM and then develop in vitro diagnostic kits for lung cancers that optimize these biomarkers to establish patient-specific TKM for further treatment.

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Code: **BIO.P-239**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Live cell-based sensor for detecting biological signal molecules

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Signaling molecules mediate communication between cells in vivo and play key roles in regulating intracellular function, metabolism, and cell fate. Detecting signaling molecules is significant for understanding these biological event. We present new tools to monitor signaling molecules using living cells, which is genetically encoded fluorescent sensor based on fluorescent trans-localization by intein-mediated reactions. The approach is based on the generation of functional signal peptide by intein-mediated splicing or cleavage reaction which is activated in response to external stimuli. First, we built a model system to use rapamycin-induced hetero-dimerization of FKBP and FRB. And then we constructed a live cell based sensing system to monitor the influx of Ca^{2+} , an important intracellular signaling molecules related to various cellular events, using split-intein conjugated calmodulin and calmodulin binding domain. The sensing system successfully reported the change of intracellular Ca^{2+} levels induced by ionophore or histamine. Finally, the sensing of corticosterone, which affects various physiological responses, was also carried out using glucocorticoid receptor protein. This live cell-based sensing systems can be engineered to report various cellular events of interest in biologically relevant environment and can be used for various application such as drug screening and disease mechanism study.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-240**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Redox-tuning of Small Molecules to Develop Chemical Regulators for Multiple Pathogenic Elements in Alzheimer's Disease

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Various pathogenic factors [*e.g.*, metal ions, metal-free amyloid- β ($A\beta$), metal-bound $A\beta$ (metal- $A\beta$), free radicals] are observed to be inter-related leading to the pathogenesis of Alzheimer's disease (AD). In order to regulate their complex interactions, the development of chemical reagents targeting such multiple components has received significant attention. Herein, we report that tuning the redox properties of small molecules is key to inventing effective chemical regulators towards the actions of pathological elements found in AD. In our newly prepared chemical series, **compound 1** with the lowest oxidation potential, is able to modulate the aggregation of both metal-free $A\beta$ and metal- $A\beta$ as well as scavenge free radicals. Our biochemical and biophysical studies illuminate that the noticeable reactivities of **1** towards metal-free $A\beta$, metal- $A\beta$, and free radicals can be achieved *via* peptide oxidation/degradation and ligand oxidation. **Compound 2**, which indicates a relatively higher oxidation potential than **1**, alters Cu(II)- $A\beta_{42}$ aggregation, whereas **compound 3**, which is hardly oxidized, shows no reactivity with metal-free and metal-treated $A\beta$ as well as free radicals. Overall, our studies demonstrate that the redox properties of small molecules can determine their regulatory reactivities against multiple factors related to AD pathogenesis.

Conference Date: October 18~20, 2017

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Code: **BIO.P-241**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A catecholamine neurotransmitter towards pathogenic features found in Alzheimer's disease

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Information on interactions between dopamine and multiple pathogenic factors of Alzheimer's disease (AD) [*i.e.*, amyloid- β ($A\beta$), metals, reactive oxygen species (ROS)] is very limited; thus, despite a suggested link of dopamine to AD pathology, it is difficult to elucidate its influence on AD pathogenesis. Herein, we report dopamine's direct interactions and reactivities with both metal-free $A\beta$ and metal-bound $A\beta$, along with its effect on the activation of proteins capable of controlling inflammation as well as oxidative stress. Moreover, our studies of a new chemical library, designed through structural variations of dopamine, identified that dopamine's oxidative cyclization with concomitant ROS production could be essential for controlling $A\beta$ aggregation and $A\beta$ -induced cytotoxicity. Detailed biochemical, biophysical, and biological investigations regarding how dopamine is able to modulate multiple AD pathogenic features will be presented. Our overall studies provide new insight into a novel role of a catecholamine neurotransmitter, dopamine, in AD pathology.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-242**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Sensitive and Specific MicroRNA Detection in a Single Neuronal Cell Using Atomic Force Microscopy

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MicroRNAs (miRNA) are small, non-coding RNAs that control the translation of messenger RNAs, thereby regulating critical aspects of plant and animal development. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Visualization of miRNAs has emerged as an important topic in biomedical fields. Therefore, accurate visualization of miRNAs at the single-cell level is of great interest due to their heterogeneity among cell population. Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray, real-time RT-PCR and in-situ hybridization. Especially, In situ detection of intracellular miRNAs requires simple sample preparation, without cell lysis and RNA isolation, and provides additional information on the subcellular localization of miRNAs. However, conventional tools are not easy to detect high spatial localization and sensitive detection of miRNAs. Therefore, a new approach for miRNA detection tool is atomic force microscopy (AFM). AFM has been extensively used to observe interaction of molecules and manipulate biomolecules in the physiological conditions at the single-molecule level. Because AFM has high lateral resolution of sub-nanometer, the nanoscale distribution of individual molecules on the sample surface could be imaged. Here, we established an AFM-based miRNA quantification and distribution method with no requisite of labeling for modification of miRNAs. In this research, visualization of a specific miRNAs in a cultured neuronal cell is measured by force-based AFM and help to understand functions of miRNA in depth.

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Surface structure of Alpha-synuclein oligomer studied by force-based 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 misfolded proteins 'Amyloid-beta ($A\beta$)' and 'Alpha-synuclein (α -syn)' at each of the disease. It is known that $A\beta$ and α -syn 'oligomer state', which represent intermediates in the fibril formation process may be primarily responsible for pathogenesis. And growing evidence suggests that $A\beta$ and α -syn might exist in one oligomer and promote the aggregation of one another in AD/PD pathology causing the disease to worsen further. However, studies of $A\beta$ and α -syn mixture oligomer have been sparse and indirect. Here, oligomer surface information could be characterized at the single-molecule level by AFM (Atomic Force Microscopy) and AFM tip modification process. With the AFM imaging mode and force mapping mode, morphology image of oligomer and surface information can be obtained with each protein antibody-tethered tip. And with the AFM tip modification process, Dendron-coated surface of the tip has an ample spacing inducing to a single interaction between the tip and oligomer. This research is able to overcome the limitations of traditional ensemble averaging methods and analyze in a new way that they did not.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Surface Structure of Amyloid beta (A β) Characterized by Atomic Force Microscopy

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Alzheimer's disease (AD) is one of the most prevalent severe degenerative neuronal diseases afflicting our elderly population. AD has been verified as a protein misfolding disease due to the accumulation of abnormally folded amyloid beta (A β) into the human brain. A β is considered to play a causal role in the development and progress of AD, but its molecular structure remains unclear. Here, we have used AFM to reveal the surface structure of A β . The observed specific interaction between A β and both C/N-terminal specific antibody suggests a surface structure model in which both N-terminus and C-terminus are exposed at the surface.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Microarrays on A Dendron-Modified Surface and Metal-Enhanced Fluorescence Nanoparticles Improving Sensitivity for MicroRNAs

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MicroRNAs(miRNAs) are small noncoding single-stranded RNAs(~22nt) that are involved in post-transcriptional modulation. The miRNA expression is associated with many diseases such as cancer, Alzheimer's disease, myocardial disease. miRNA is 22mer shorter than general RNA, thus miRNA is amplified by PCR. In particular, the role of miRNAs in cancer has been extensively studied. miRNA analysis can be useful for early diagnosis or treatment of diseases. Currently, Polymerase Chain Reaction (PCR) is a standard method to detect miRNA. However, it causes error in amplification process and analysis sensitivity is relatively low. In order to overcome the limitations of the conventional technology, I will improve the sensitivity more than 100 times using metal-enhanced fluorescence nanoparticles and microarray. Here we suggest new approaches to supersensitive analysis of miRNA using metal-enhanced fluorescence (MEF) nanoparticles and microarray. To detect miRNA, we use S9.6 antibody that is DNA/RNA hybrid-specific mouse monoclonal antibody. This approach is expected to perform parallel analysis with detection sensitivity increased several hundred times more than the conventional methods.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-246**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Quantitative Analysis of Neuronal Proteins Using Atomic Force Microscopy

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Proteins perform a vast array of functions within living organisms, including catalyzing metabolic reactions, DNA replication, responding to stimuli, and transporting molecules from one location to another. Detection of proteins of low expression level is frequently important, because a certain proteins exist at very low level during the early stages of cell development. In particular, neuronal proteins of the kind play a key role in the regulation of development and synaptic plasticity of neurons. Conventional methods to analyze proteins include western blotting, ELISA, and immunofluorescence. However, these tools suffer from poor limit of detection, and cannot visualize proteins in high lateral resolution. Therefore, atomic force microscopy (AFM) is a good candidate to overcome the hurdles. AFM is a powerful tool to show information about the distribution of the biomolecule. Using the mapping capability of AFM, it is possible to obtain a map the distribution of a specific protein in a nanometric resolution. And we can count the copy number of protein in a sample solution. In the congress, we present our effort to demonstrate such capability of AFM.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-247**

Area: Life Chemistry

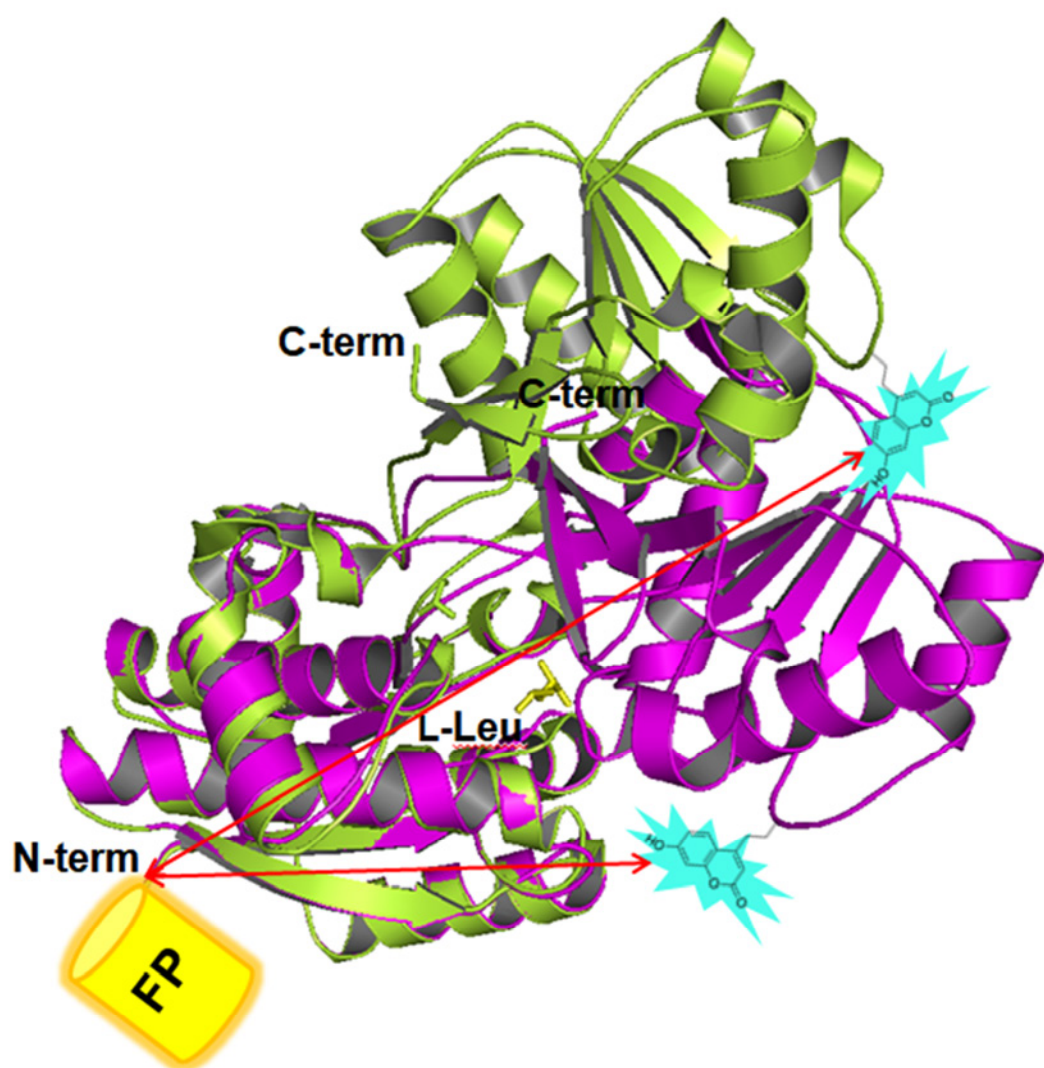
Type: Poster Presentation, Time: THU 11:00~12:30

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 report, a leucine binding PBP was engineered to detect 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 yellow fluorescent protein (YFP) was fused to its N-terminus as a FRET acceptor. When CouA was incorporated into 178 position, the sensor protein showed 2.5-fold increase in FRET ratio. By engineering the protein, its substrate specificity was significantly improved, 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-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.



AMERICAN CHEMICAL SOCIETY

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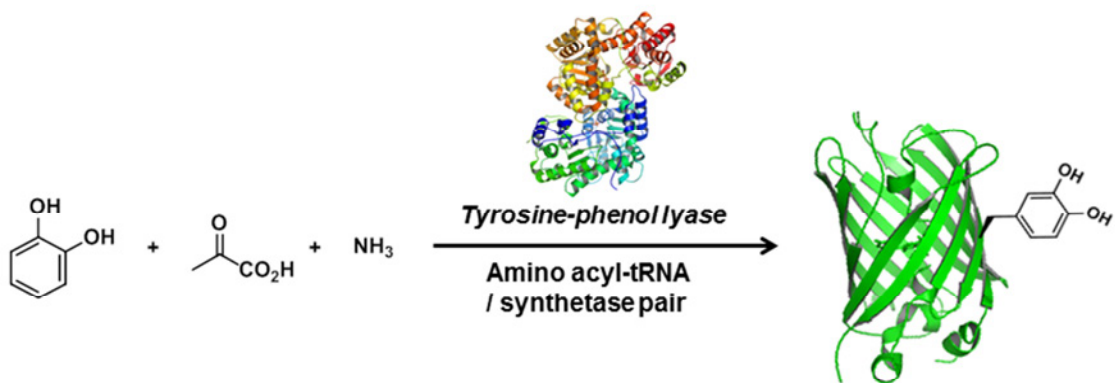
Type: Poster Presentation, Time: THU 11:00~12:30

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

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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



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **BIO.P-249**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Misfolded Z-type α_1 -Antitrypsin Proteins Induce Oxidative Stress

Hana Im^{*}, JAEYEON LIM

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Protein misfolding and aggregation is associated with various human degenerative diseases, including type II diabetes, Alzheimer's, Huntington's, and Parkinson's diseases. Accumulation of misfolded Z-type variant of human α_1 -antitrypsin protein in the ER leads to persistent ER stress and subsequent cell death, leading to liver cirrhosis. A *Saccharomyces cerevisiae* ORF-deletion library was screened for the response elements to accumulation of misfolded Z-type α_1 -antitrypsin protein. Several deletion mutants of redox regulator genes aggravated Z-type α_1 -antitrypsin-induced cytotoxicity. We have also shown that overexpression of Z-type α_1 -antitrypsin caused cellular oxidative stress by dichlorofluorescein assays. Z-type α_1 -antitrypsin-producing cells became vulnerable to further oxidative challenges with low concentrations of hydrogen peroxide. Treatment with antioxidant chemicals, such as ascorbic acid, N-acetylcysteine, or butylated hydroxyanisole protected yeast cells from Z-type α_1 -antitrypsin-induced cytotoxicity. Our data all together provide further insight on cell defense mechanism against protein folding problems, and suggest future therapeutic applications. This work was supported by grants from the National Research Foundation of Korea (KRF-2015R1D1A1 A01058206).

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **BIO.P-250**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Cyclophilins protect yeast cells from freeze-stress

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Exposure to freezing temperatures are one of the major challenges faced by many organisms. Low temperatures reduces protein folding rates and induces the cold denaturation of proteins, necessitating aid from chaperones. Thus, a yeast ORF-deletion library lacking individual chaperones were screened for reduced freezing tolerance. In total, 19 of 82 chaperone-deleted strains tested were more sensitive to freeze-thaw treatment than wild-type cells. The freeze survival of the chaperone-knockout strains was increased in the presence of 20% glycerol, suggesting that ice crystal formation during freezing may be one of the major causes of cell death. Among those, peptidyl-prolyl cis-trans isomerases (PPIases) including cyclophilins, were the most frequently identified. At low temperatures, peptidyl-prolyl isomerization is a rate-limiting step in protein folding, and folding intermediates, which are prone to protein aggregation, tend to accumulate. Overexpression of PPIases protected β -galactosidase protein from cold denaturation. Purified PPIases also facilitated the refolding of a slow-folding substrate protein in vitro. These results suggest that the identified PPIases enhance cold survival of cells by preventing cold-induced protein denaturation and promoting protein folding. This work was supported by grants from the National Research Foundation of Korea (KRF-2015R1D1A1 A01058206).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-251**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Component interactions between hydroxylase and auxiliary enzymes from *Methylosinus sporium* strain 5

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The studies of sMMO have focused on *Methylococcus capsulatus* Bath (*M. capsulatus*) and *Methylosinus trichosporium* OB3b (*M. trichosporium*) for last 25 years, but mechanistic studies are still needed in order to understand methane conversion to methanol. Enzymatic mechanisms and chemical interactions of sMMO which belong to bacterial multicomponent (BMM) systems are required to understand. To date, findings are retarded due to the difficulties of complex formation during enzymatic studies. This implies that MMOB and MMOR controls the oxidation reactions of hydroxylase. These studies will address those questions to develop new enzymes for the production of methanol from methane gas. The structure and function of the active site (di-iron) will be studied using rapid freeze quench (RFQ) spectroscopic methods. The activation energy to break the C-H bond in methane is significantly high (104.9 kcal/mol). Therefore, intermediate structures during enzyme catalysis need to be elucidated when bound to substrate during the catalytic cycle. In addition, electron transfer mechanisms will be performed to get catalytic activities. X-ray crystallography of MMOH-MMOR will provide insight into electron transfer pathways. Structural and functional consequences from basic studies will be applied in *E. coli* or other natural bacterial systems for practical use. MMOB and MMOR interactions with engineered enzymes will accelerate the oxidation of specific substrates. The chaperon proteins will be modified to enhance performance in heterologous systems via biochemical and molecular biology methods.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-252**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Heterometal coordination to concanavalin A and its cadmium substitution

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Rapid methods for the detection and clinical treatment of human norovirus (HuNoV) are needed to control foodborne disease outbreaks, but reliable techniques that are fast and sensitive enough to detect small amounts of HuNoV in food and aquatic environments are not yet available. We explore the interaction between HuNoV and concanavalin A (Con A), which could facilitate the development of a sensitive detection tool for HuNoV. Biophysical studies including hydrogen/deuterium exchange (HDX) mass spectrometry and surface plasmon resonance (SPR) revealed that when the metal coordinated region of Con A, which spans Asp16 to His24, is converted to nine alanine residues (mCon AMCR), the affinity for HuNoV (GII.4) diminishes, demonstrating that this Ca²⁺ and Mn²⁺ coordinated region is responsible for the observed virus-protein interaction. The mutated carbohydrate binding region of Con A (mCon ACBR) does not affect binding affinity, indicating that MCR is a major region of interaction. The results further contribute for the development of a HuNoV concentration tool, Con A-immobilized polyacrylate beads (Con A-PAB), for rapid detection of genotypes of genogroup I and II (GI and GII). This method offers many advantages over currently available methods, including a short concentration time. Norovirus can be detected in just 15 minutes with 90% recovery through Con A-PAB application. In addition, this method can be used over a wide range of pH values (pH 3.0–10.0). Overall, this rapid and sensitive detection of human norovirus will aid in the prevention of virus transmission pathways and the method developed here may have broad applicability for other foodborne viral infections.

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Code: **BIO.P-253**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Optimal growth and development through salt-defense mechanisms in *Suaeda glauca*

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Mechanistic studies of halophytes are urgent areas of agricultural research due to the increase in saline-contaminated lands and irrigated fields worldwide. The halophyte, *Suaeda glauca* (*S. glauca*), has many advantages in terms of biomass and saline elimination due to its large mass and well-developed phenotype on seashores, although its mechanistic features and growing specificities still require systematic investigation. Preliminary studies have indicated that secondary metabolites, including alkaloids, are key metabolites for achieving salt tolerance and that indole derivatives retard the inhibition of growth and development in halophytes. Metabolomic studies have validated that indole-3-carboxylic acid (ICA) and indole-3-acetic acid (IAA) accumulate in halophytes under saline conditions. In this study, *S. glauca* were cultivated under various saline concentrations (0–400 mM) in Hoagland's solution in the absence or presence of indoles to elucidate physiological features via systematic monitoring. The results confirmed that the optimal growth and development of *S. glauca* in 50 mM NaCl, and the morphology, such as the number of branches, shoot lengths, and fresh and dry weights, were improved by exogenous ICA treatment. The cation concentrations in roots, shoots and leaves were investigated to examine the ionic imbalance in response to saline treatment, and the results demonstrated that sodium ions accumulated to high concentrations in leaves. The levels of calcium and potassium ions in root were maintained at 50 mM NaCl, an optimal growth condition, but ICA and IAA did not regulate the ion concentrations. This study demonstrates the optimal growth conditions in saline for *S. glauca* and the phenotypic regulation of ICA, although the ionic imbalance was controlled by genetically programmed physiology. These results will provide valuable information for bioengineering based on the high levels of biomass in *S. glauca* to achieve salt tolerance in glycophytes and halophytes.

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Code: **BIO.P-254**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Catalytic roles of zinc finger proteins with structural integration

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Zinc finger (ZF) proteins use zinc as a structural co-factor and are often involved in nucleic acid recognition and binding. Although zinc is typically thought to be the physiologically relevant transition-metal ion for ZF protein function, there is evidence that other metal ions, including iron, may replace zinc under certain conditions. Studies focused on the roles of metal coordination and DNA binding for two specific ZF proteins: ST18 (suppression of tumorigenicity 18) and ZIF268 (zinc interacting factor 268) will be presented. ST18 is a non-classical ZF that belongs to the NZF/MyT family of ZFs. It contains six ZF domains, each of which has a Cys2His2Cys motif. The biological function of ST18 is not well understood; however, there is some recent evidence that ST18 regulates inflammation and apoptosis by regulating gene expression of tumor necrosis factor-alpha (TNF- α). We have been studying constructs of ST18 that contain the Cys2His2Cys domains, and have obtained evidence for zinc binding. These studies along with DNA binding studies with the TNF- α promoter will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-255**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Wash-free labeling of target proteins and the use of photochemical handles in live cells

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Monitoring protein functions, interactions and movements in living cells is critical for understanding their roles in biological system. In particular, fluorescent probes allow detection of molecular interactions, mobility and conformational changes of proteins in live cells with high temporal and spatial resolution. In this study, we utilized *Npu* DnaE split-intein mediated protein trans-splicing (PTS) reaction for site-specific fluorescent labeling of target protein. The large N-intein (I_N), is expressed using DNA recombinant technology as a fusion to a target protein. The smaller C-intein (I_C) carrying a quencher and a fluorophore, Q-Ic-Fl, was chemically synthesized and delivered into mammalian cells. We first tested fluorescent labeling of model membrane anchored proteins on live cells using engineered *Npu* DnaE split-intein based PTS reaction. The labeling reaction occurred in two different modes. First, the fast and instant labeling occurred via specific binding of two split-intein fragments, and second, more stable and irreversible labeling occurred via covalent bond formation through split-intein mediated PTS reaction. We next showed fluorescent labeling of cytosolic protein using a fluorescence-quenched peptide, Q-Ic-Fl. This approach enabled wash-free labeling of target cytosolic proteins. Finally, we attempted to photo-trigger the labeling reaction in live cells using Q-iso Ic-CPP-Fl. The photo cage was removed by irradiation to restore functional intein from the photocaged iso-Ic. The activated intein carried out the labeling reaction, successfully. This approach can be used as a tool to monitor the functions and locations of target proteins in live cells with spatiotemporal resolution.

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Code: **BIO.P-256**

Area: Life Chemistry

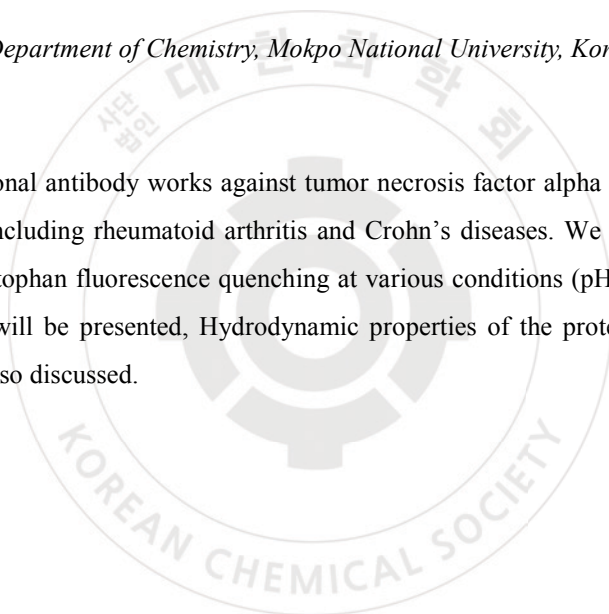
Type: Poster Presentation, Time: THU 11:00~12:30

Conformational stability of a TNF- α monoclonal antibody investigated by steady-state fluorescence quenching

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Infliximab is a monoclonal antibody works against tumor necrosis factor alpha (TNF- α) for treatment of autoimmune diseases including rheumatoid arthritis and Crohn's diseases. We initiated characterization of the antibody by tryptophan fluorescence quenching at various conditions (pH, storage period, reducing agent etc) and results will be presented, Hydrodynamic properties of the protein estimated by velocity sedimentation will be also discussed.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-257**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Colorimetric sensor applications for agro-food fields

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A naked-eye detective colorimetric sensor has been a major concern in the postharvest technology of agricultural products. From harvest immediately after to consumption, postharvest technology based on storage and distribution is an effective method to minimize a property loss and to sustain the high quality of safe agricultural products. Especially, colorimetric sensors could communicate with consumers through colors which include the information of agricultural products, such as quality and ripeness. In addition, this sensor offers the time-saving convenience for the final purchasing decision as well as can be used as a marketing tool to elevate the value of product. Monitoring the high quality of agricultural products with non-destructive methods is employed by on-packaging smart sensors which are sensitive to fruit aroma and temperature. Fruit aroma sensitive colorimetric chemosensor utilizing pH dye molecules is designed for the determination of apple ripeness. A temperature-response colorimetric sensor is fabricated by thermochroic materials base on the electron transfer between acceptor and donor, as like HITE beer label. Non-destructive sensor applications by chemical approaches will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-258**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A small periplasmic protein with a hydrophobic C-terminal residue enhances DegP proteolysis as a suicide activator

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DegP is a highly conserved protease that performs regulated proteolysis to selectively remove misfolded proteins in the periplasm of *Escherichia coli*. Binding of misfolded proteins is known to be the main mechanism of DegP activation, but it is unknown whether any native proteins can alter DegP activity. Here, we show that a small periplasmic protein, YjfN, which is highly upregulated by the Cpx envelope stress response, functions as a “suicide activator” for DegP and promotes efficient degradation of misfolded proteins. YjfN readily binds to and is degraded by DegP, for which a hydrophobic C-terminal residue and transient unfolding of YjfN are critical. YjfN also activates DegP in trans while it is being degraded, and accelerates degradation of a denatured outer membrane protein, OmpA, that is not easily recognized by DegP. Although YjfN also prevents OmpA aggregation, the trans-activation effect is mainly responsible for efficient OmpA degradation. Overexpression of YjfN enhances the viability of cells in misfolded protein stress that is induced by the presence of a less-active variant of DegP at high temperature. Collectively, we suggest that YjfN can enhance DegP proteolysis for relieving envelope stresses that may generate toxic misfolded proteins.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-259**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of a new method for finding protease substrates and its application to study the protein degradation

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Proteases are one of the largest group of enzymes. Their deregulation is associated with pathogenesis of many human diseases due to the critical function of proteases in cellular processes, including protein quality control by degrading unfolded or misfolded proteins. The tools for searching the general protease substrate(s) are limited. So the development of a method that allow identification of general protease substrate(s) is a challenge of high interest, since it will not only enhance our understanding of the cellular functions of proteases, but will allow identification of targets for development of novel therapeutics. In the system developed in our laboratory, proteases that have serine, cysteine and threonine residues in the active sites form an acyl-enzyme intermediate in the first step by combining with the substrate N-term fragment. Then, intermediates are hydrolyzed to complete cleavage in a general reaction. In the second step, if there are more of better nucleophiles than H_2O , they will form covalently-linked products with the substrate N-terminal fragment. These peptides are selected and sequenced by LC-MS/MS. Through this method, we will be able to identify the original substrate. This new method to profile substrate is named Trapping Proteolysis Intermediates (TraPI).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-260**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Effect of ERLBD302-552 on the amyloid fibril formation of α -synuclein

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α -Synuclein (α Syn) protein of Parkinson's disease patient undergoes conformational change to form amyloid fibrils as insoluble deposit. In our previous study, we have constructed the plasmid ERLBD302-552/pET28 and overexpressed the His-tagged ERLBD302-552 protein by IPTG induction using BL21(DE3). In the present study, we examined the process of amyloid fibril formation of α Syn in the presence of His-tagged ERLBD302-552 in vitro. We also made the fusion construct ERLBD-L23- α Syn/pET28a by cassette ligation. Finally we discuss the function of ERLBD302-552 on the amyloid fibril formation of α Syn based on the ThT fluorescence kinetics of fusion protein.

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ultrastable Synthetic Host-Guest Interaction Based Supramolecular Latching System as a Versatile Bioimaging Tool in Chemical Biology

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Protein-ligand binding pairs such as streptavidin-biotin (SA-BT) have been used as an efficient tool for fluorescence-based cellular imaging to examine the function, structure and localization of proteins of interest. However, the SA-BT based methods suffer from intrinsic drawbacks including their large size, interference of endogenous biotinylated protein and enzymatic degradations. Herein, we demonstrate that the supramolecular latching system based on the ultrastable synthetic host-guest molecules, cucurbit[7]uril (CB[7]) and adamantyl (AdA) or ferrocenyl ammonium (FcA), can be exploited for location-specific protein visualization by employing a variety of different conjugation methods.¹ Proteins of interest were labeled with AdA by using location-specific labeling methods and selectively visualized upon treatment of cyanine 3-conjugated CB[7] (Cy3-CB[7]),² with no interference from endogenous biomolecules, which enables us to generate clear fluorescence images for accurate and precise protein analysis using fluorescence microscopy. This ultrastable synthetic binding pair system using CB[7] can be a new tool for cell imaging. Additionally, this newly developed synthetic system can be used with conventional SA-BT based systems, which may enable us to visualize proteins, with high resolution, involved in various biological processes such as protein-protein interactions and organelle communications.

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Th role of NUDT9 in hypoxia-inducible factor pathway

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Although numerous kinases have been reported to regulate HIF-1 α stability and activity, few phosphatases are known to be involved in HIF-1 α regulation. In this study, we report that ADP-ribose (ADPR) pyrophosphatase, nudix hydrolase 9 (NUDT9) negatively regulates HIF-1 α accumulation by modulating AMP-activated protein kinase (AMPK) signaling pathway. Knockdown of NUDT9 activates transient receptor potential cation channel subfamily M Member 2 (TRPM2), resulting in Ca²⁺ influx mediated activation of calcium/calmodulin-dependent protein kinase kinase (CAMKK β). AMPK activation by CAMKK β is shown to enhance HIF-1 α accumulation and the possible downstream effector for AMPK is identified. Our finding provides insights into the roles of NUDT9 phosphatase as additional, discrete modulator of hypoxia stimulated HIF-1 α accumulation through different signaling pathways.

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Hair analysis in various pH conditions with FTIR microspectroscopy

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In this research, natural and intact hair is used and experiments are performed within pH range from 1 to 12. Given that nitrogen oxide is the major cause of acid rain, nitric acid was used for making acidic solution and for the basic one, normal potassium hydroxide was used. Hair was paraffin-embedded and microtome was used to get the cross-section. In each pH, IR spectrums and cross-section images are obtained with FT-IR microspectroscopy and surface images with SEM. Since a hair fiber can be divided into outer layer(cuticle) and inner part(cortex), comparisons between these two parts are also made in each part. Especially in IR analysis, Amide I band was used for studying secondary structures of protein. From the controlled experiments, we will present how the human hairs can be affected and the detailed analysis in each pH condition will be presented.

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Deposition of Single and Multi component ECM and Investigate mechanical properties of ECM vesicles

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The extracellular matrix (ECM) has important roles in regulating the development, function and homeostasis of all eukaryotic cells. Essentially, binding of ECM molecules to integrin induces ECM unfolding, thereby spontaneously promoting interactions and fibril assembly. ECM fiber can be coated on GUV by negative charge. Giant unilamellar vesicle (GUV) is a simple model of complex cells. For fibrillogenesis of ECM such as Laminin and Fibronectin outside of vesicle, vesicles were made with PS lipid with negative charge ahead. Then GUV were incubated with ECM dimer at 37°C during 12hrs. As a result, Single and Multi component ECM coated vesicle was obtained. We analysed structure of binding ECM and investigate mechanical properties by micropipette aspiration. Fibronectin bind themselves by stretching their length and wholly cover on GUV but Laminin bind together by their arms (not stretching) so not evenly cover on GUV. Multi component of ECM will be a good model of cell because there is no distortion and modulus is similar to real cells. Laminin increase area expansion modulus and this GUV can be reached near by real cell's modulus of mechanical properties.

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Glycan-density dependent binding of pathogenic proteins and cells

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Pathogens express various glycan-binding proteins (adhesins or lectins) for infection of humans. For example, *Helicobacter pylori* strains express SabA and BabA proteins on their surface to bind sialyl Lewis x and Lewis b on epithelial cells for infection. Another important pathogenic lectin is Hemagglutinin expressed on influenza virus. This viral lectin recognizes NeuNAc• 2,3Gal or NeuNAc• 2,6Gal on epithelial cells. Thus, understanding of pathogenic protein-glycan interactions is of great importance to discover diagnostic and/or therapeutic agents. To rapidly analyze interactions between pathogenic proteins and glycans, we have developed carbohydrate microarrays containing a number of glycans in a density-dependent manner. By using the microarrays, we have analyzed pathogenic protein-glycan interactions. It was found that pathogenic proteins recognize multivalent glycans on the surface more tightly compared to monovalent glycans. We also made an attempt to detect intact pathogens using glycan microarrays.

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Screening of carbohydrates that elicit immune responses using glycan microarray

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Lectins expressed on the immune cell surface associate with pathogenic cell surface glycans, the process that leads to stimulation of immune responses to pathogens. Mouse SIGN-R1 (SIGN-related 1) is known to recognize mannose-rich and fucose containing glycans in a Ca²⁺-dependent manner. When SIGN-R1 binds to glycans on bacteria or viruses, glycan antigens enter cells via lectin-mediated endocytosis to stimulate immune activation. In this study, we applied glycan microarrays containing various glycans to rapidly identify glycans that elicit cell surface lectin-mediated cellular responses. Because binding of glycan ligands to SIGN-R1 on the cell surface leads to production of reactive oxygen species (ROS), the functional glycans on the microarrays are rapidly identified by using a ROS-selective fluorescent probe (PF1). Glycan microarrays were created by attaching 31 unmodified glycans on the hydrazide-coated glass surface. SIGN-R1 expressing cells that were pre-treated with PF1 were applied to the glycan microarrays and the fluorescence intensity of the cells was then determined by using a confocal fluorescence microscopy or a microarray scanner. The results of microarray experiments showed that Man and Fuc possessing glycans stimulate ROS production, a phenomenon that was blocked in the presence of a ROS scavenger or an NADPH oxidase inhibitor. The present study demonstrated that glycan microarrays serve as a useful tool to uncover functional glycans that enhance cell surface lectin-associated cellular responses.

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Discovery of Lectin-selective Ligands Using Carbohydrate Library Microarrays

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Binding of lectins to glycans, present in cells in the form of glycoconjugates such as glycoproteins, glycolipids and proteoglycans, is a critical process that triggers a number of physiological and pathological events. It is known that lectins have distinctive but overlapping glycan binding properties. To elucidate biological events promoted by lectin binding to glycans, ligands that interact with one lectin but not with other lectins that have overlapping binding properties are in high demand. Ligands with such characterizations can be used as chemical probes to modulate specific glycan-lectin interactions. Plant lectins have been widely employed as biological research tools and diagnostic agents. It has been shown that plant lectins are capable of inducing apoptosis in various cancer cells, even though the molecular mechanism underlying apoptotic cell death remains unclear. Because of their biological and biomedical significance, binding specificities of plant lectins have been extensively examined. In this study we synthesized a library consisting of 55 hydrazide-linked mono- and disaccharide analogs and prepared microarrays containing the analogs. The microarrays were then employed to identify lectin-selective ligands. The microarray study shows that two disaccharide analogs selectively bind to *S. tuberosum* lectin (STL) and wheat germ agglutinin (WGA). Two compounds in this library were observed to display selective binding to plant lectins and to possess the ability to selectively block binding of the lectins to mammalian cells. The results of cell studies also indicate that two compounds selectively block binding of STL and WGA to mammalian cells unlike a natural ligand LacNAc that suppresses binding of both STL and WGA to cells. This study demonstrates that carbohydrate analog microarrays allow for rapid identification of lectin-selective ligands. Because many plant lectins modulate various biological processes, including apoptosis, it is expected that the method developed in this effort can be utilized to develop ligands that serve as chemical probes to modulate plant lectin-mediated biological processes.

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Effects of Charge and Ligand Structure of Gold Nanoparticles on Mammalian Cells

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Gold nanoparticles (AuNP) has been widely used and gained abundant interest due to its optical, ease of quantification in a biological system, and size/ shape dependent photothermal properties. In addition, due to the biocompatibility and flexibility of surface functionalization, AuNP has been actively studied for nanotechnology with the development of nanomaterials in a wide range of medical fields. However, the effects of physical properties of AuNP on biological effects have not yet been clarified, and it is also true that some studies have disagreed. Therefore, for safe usage of AuNPs in biomedical application, it is important to study systematically how physicochemical properties of gold nanoparticles change their biological interactions. Among many variables, we here focused on the effect of surface chemistry, charge and structure of ligands. For a systematic approach, we prepared mono-dispersed AuNPs of series of charges ranging from -42.8 ± 11.8 mV to $+41.8 \pm 3.8$ mV with various functional groups based on a sequential ligand exchange method. Then various biological assays were performed to measure the effects of each AuNPs on cell viability as well as on various cellular functions of mammalian cell lines. Uptake efficiency of AuNPs by mammalian cells and the subsequent changes of cell morphologies and cytoskeletal structures were also monitored. This study showed that the anionic and neutral AuNPs did not show cytotoxicity, whereas the cationic AuNPs were classified as toxic and non-toxic according to their ligands. While all the cationic AuNPs tested were more effectively internalized by mammalian cells compared with anionic or neutral AuNPs, only the cytotoxic MUAM-AuNP showed inhibitory effects on the DNA replication and on the formation of actin filament. As MUAM carries both cationic head groups and hydrophobic moieties, we suspected that this structural characteristics of MUAM could be the origin of cytotoxicity. In order to further verify this idea, we prepared modified CP1-AuNP (RRRGYKC₁₁C-AuNP), by introducing hydrophobic moiety and the cytotoxic effect of modified CP1-AuNP was studied. Introduction of a hydrophobic moiety on the AuNPs surface resulted in increased cytotoxicity. The results

showed that not the charge of the AuNPs but the structure of the ligand was an important factor determining the biological effects of AuNPs. This work also proposed that properly designed cationic AuNPs could make a good candidate for low toxicity gene-delivery materials.



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Binding Properties of the N-Terminal and the C-Terminal Domain of Riboflavin Synthase

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To study the biochemical characteristics of RibE from *Photobacterium leiognathi*, the recombinant plasmids of pQE containing the truncated genes coding for the half of N-terminal and the C-terminal of RibE, as well the whole RibE have been constructed, respectively. The RibE has the amino acid homology with riboflavin synthase from *Escherichia coli*. Riboflavin synthase catalyzes the formation of one molecule of each riboflavin and 5-amino-6-ribitylamino-2,4-pyrimidinedione from two molecules of 6,7-dimethyl-8-ribityllumazine. Riboflavin synthase from *Escherichia coli* was shown to be a homotrimer of 23.4 kDa. The most remarkable feature is the intra-molecular sequences similarity between the N-terminal and the C-terminal half of riboflavin synthase from *Escherichia coli*. Similarly, the proteins have amino acid identity between the N-terminal and the C-terminal domain halves of RibE from *Photobacterium leiognathi*. The truncated 6X-His tagged proteins of the N-terminal and the C-terminal domain, as well as the whole RibE were purified by binding Ni-column followed by elution with imidazole. The binding properties of the truncated proteins as well as the whole RibE were examined by absorbance and fluorescence spectroscopic analysis with 6,7-dimethyl-8-ribityllumazine and riboflavin. This work was supported by IPET (313058051 HD020).

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Delivery of Fibronectin into fibroblast via Small Unilamellar Vesicles for wound healing

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Fibronectin(FN) is a key component of extracellular matrix, playing a primary role in tissue repair and cell growth. It exists in two forms: plasma fibronectin and cellular fibronectin. In this study, plasma fibronectin was used and coated on negatively charged lipid vesicles, known as small unilamellar vesicles(SUVs). Our goal was to observe the effect of FN-SUV on cell growth and wound healing. SUVs were fabricated and incubated with FN at 37°C for 12hr. Then the complex of FN-SUVs was delivered into fibroblast. The observation of cell growth with and without the presence of FN-SUV was conducted in every 12hr. The results show that the rate of cell growth is faster with the treatment of FN-SUV comparing to without the treatment. Additionally, this FN-SUV also assists wound healing.

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Area: Life Chemistry

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The genetic association with three endocytosis-related genes and Alzheimer's disease

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Alzheimer's disease (AD) is the most common type of dementia among the people more than 65 years-old. Many reports have been performed to investigate the pathogenesis of AD. Recently, several reports showed that defects in endocytic membrane trafficking and vesicular transport were associated with AD. The endocytosis was essential for releasing neurotransmitters, as increasing membrane retrieval and neuronal growth factor receptors. For these reasons, we examined the association between endocytosis-related gene polymorphisms and risk of AD with 144 cases and 335 controls. We evaluated the association between three polymorphisms and AD using meta-analysis. Our results showed the significant association between endocytosis-related gene polymorphisms and risk of AD. Especially, the *PICALM* rs3851179 polymorphism was detected decreasing risk for AD. It may be a protective genetic factor to progression of AD. However, the other polymorphisms indicated increasing risk factor to AD. In conclusion, the three endocytosis-related gene polymorphisms are potential risk factor with pathogenesis of AD.

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Mitochondria-Penetrating Peptide (MPP) for Hydrophobic Drug or dye Conjugate (MPDC) for efficient antitumor therapy

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Recently, targeting mitochondria is a promising strategy to improve chemotherapy efficiency by reducing side effects. Mitochondria penetrating peptide (MPP) has been worked to offer highly efficient gene or drug delivery. Most MPPs consist of alternative positive charged amino acids such as arginine (R) and lysine (K) and lipophilic amino acids such as phenylalanine (F) or cyclohexylalanine (Fx). In here, mitochondria targeting peptide can be achieved with hydrophobic drug or dye acted as lipophilic amino acids. These mitochondria targeting peptides which are short and highly positive peptides with anticancer drug, camptothecin (CPT) and IR-780 has been synthesized in which the CPT and IR-780 are conjugated to peptide via thiol functional group of cysteine in peptide. It can self-assemble into nanostructure in water. First, the mitochondria targeting peptide containing IR-780 can be used for NIR imaging and photothermal therapy with laser irradiation and mitochondria targeting drug can be released via disulfide bond based on intracellular GSH concentration. These short peptides conjugated to drug exhibited target specific toxicity with antitumor efficiency also the dye conjugated peptides showed target tumor toxicity with photothermal therapy. .

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Development of simple and rapid method for detection of Aichi virus A by Ultra-Fast PCR

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Aichi viruses has been proposed etiological factors of acute gastroenteritis(GE) that occurs diarrhea and vomiting. Especially, acute gastroenteritis is increasing cause of mortality worldwide in children and the elderly. Therefore, simple and rapid detection for Aichi virus is important for prevention of infection. Previous studies reported that several diagnostic techniques such as RT-PCR, real-time PCR and nested PCR were performed for detecting Aichi virus A. These methods are expensive and time-consuming that require highly precise thermal cyclers. For these reasons, amplification techniques for detecting viruses in point-of-care testing(POCT) are required more simple, inexpensive, and rapid than previous studies. Ultra-Fast PCR is simple and movable method that performs 30 cycles within 15 min. In addition, amplification products are observed thorough the window on the top of GENECHECKER™ Ultra-Fast PCR system. A polymer chip for Ultra-Fast PCR is thin and high heat conductive. In this study, we performed detection of Aichi virus A using Ultra-Fast PCR amplification. And we compared Ultra-Fast PCR with previous studies(conventional PCR and real-time PCR). As a result, we used Ultra-Fast PCR to detect Aichi virus A and confirmed that GENECHECKER™ is able to detect Aichi virus within 25 minutes. Furthermore, Ultra-Fast PCR was amplified DNA products 1 hour faster than conventional PCR and real-time PCR. In conclusion, Ultra-Fast PCR has demonstrated simple, rapid, and efficient tool which can be available in molecular diagnosis in POCT.

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eDHFR and eDHFR_R12Y_Y100I proteins Inhibit Amyloid Fibril Formation of α -Synuclein

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Building on our previous work with FKBP-based system, we investigated regulator protein(s) for amyloid fibril formation of α -synuclein (α Syn). In the present study, *E. coli* dihydrofolate reductase (eDHFR) and its mutant (eDHFR_R12Y_Y100I) were cloned in pET28a vector to produce bacterial expression plasmids using PCR and site directed mutagenesis. Both eDHFR and eDHFR_DD (R21Y_Y100I as destabilization domain (DD)) was successfully expressed in BL21(DE3) in the presence of IPTG and purified by Ni²⁺-affinity chromatography. According to the thioflavin T (ThT) fluorescence assay, we observed that eDHFR inhibited the amyloid fibril formation of α Syn in a dose-dependent manner. It is noteworthy that the inhibitory effect of eDHFR_DD is more profound than that of eDHFR, suggesting an important role of DD as a regulator of amyloid fibril formation.

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NMR Structural analysis of syndecan-4 receptor

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Syndecan-4 is a widespread heparan sulfate proteoglycans also present in human mesenchymal cells, epithelia and endothelia, and is involved in focal adhesion assembly and cytoskeletal organization. In addition, the interaction of syndecan-4 with GFRs (growth factor receptors) is a very important factor in cancer progression and is particularly associated with resistance to treatment and therapy in breast cancer. To get a better understanding of the mechanism and function of syndecan-4, it is crucial to investigate its three dimensional structure. Syndecan-4 comprises three major sections: extracellular (ecto-), transmembrane (TM) and cytoplasmic (Cyto-) domains. It also forms a dimer like the transmembrane domain of all syndecans forms homodimers by highly conserved GXXXG motifs. The cytoplasmic domain of syndecan-4 forms twisted dimers by the presence of PIP2 (phosphatidylinositol (4,5)-bisphosphate), which induces protein kinase $C\alpha$ persistently binding and activation. Thus, the structural alteration of the transmembrane and cytoplasmic domains by binding with PKC- α and PIP2 regulates the function of the extracellular domain. We obtained pure protein samples by expressing and purifying wild type Syd4-TM (wtSyd4), mutant Syd4-TM(mSyd4) and Syd4-eTC(ecto-, TM, Cyto-), respectively, for structural studies to understand the function of syndecan 4. And their structures were investigated by various spectroscopic methods as well as solution/solid-state NMR spectroscopy.

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Development of novel antimicrobial peptides derived from Lactophorin with enhanced antimicrobial activity

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Bacteria that have Anti-Microbial Resistance (ARM) are increasing due to antibiotics abuse, nowadays and it has attracted people's attention to antimicrobial peptides (AMPs). Therefore, we studied LPcin-I and LPcin-II derived from lactophorin, a cationic amphipathic antimicrobial peptide consisting of 23 amino acids. The antimicrobial activity of alpha helical antimicrobial peptides is controlled by various factors such as net positive charge, α -helicity, and hydrophilic/hydrophobic region. So, we design YK1, YK2 and YK3 derived from LPcin-I. And among these, YK3 showed the best antimicrobial activity so we used it to develop new AMPs with a shorter length and improved antimicrobial activity. First, antimicrobial peptide was mutated to increase the net charge and amphipathicity was reduced to prevent self-aggregation. Finally, mutation to facilitate interaction with the bacterial membrane was done. finally, we designed and selected the new antimicrobial peptides YK5, YK8 and YK11 based on YK3. Designed all analogues were expressed and purified using several biophysical techniques and characterized using antimicrobial activity tests and various spectroscopic methods like MALDI-TOF MS and CD spectrometry, as well as 1D/2D solution NMR and solid-state NMR techniques in membrane environments.

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Enzymatic crosslinking of side chains generates a modified peptide, Plesiocin, with four hairpin-like bicyclic repeats

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Ribosomally synthesized and Post-translationally modified Peptides represents a unique class in natural products. Especially, macrocyclization involved in RiPP biosynthesis yields topologically diverse cyclic peptides. Cyclization via ester or amide bonds are easily found in RiPP, but crosslinking of two side chains through ester or amide is uniquely found in the microviridin class of natural products with a single consensus sequence of peptides. Here, we report plesiocin, a new microviridin-like RiPP which has a distinct sequence pattern, also can be enzymatically crosslinked via ester bonds to make a novel modified peptide, and showed strong inhibitory effect against some serine proteases. A single ATP-grasp enzyme binds to a leader peptide, of which only 13 residues are required for binding, and performs eight esterification reactions on the core peptide. We demonstrate that connectivity of side chains can be easily analyzed by the combination of tandem mass spectrometry and methanolysis of esters. We suggest that crosslinking of peptide side chains can generate diverse structure.

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Purification and Inhibition Study of Fatty Acid Synthase, A Potential Target for Anti-cancer drugs

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Fatty acid synthase (FAS) is an enzyme in the palmitate pathway that catabolizes the saturated fatty acid of 16-carbon long palmitate from acetyl-coA and malonyl-coA. Because the fatty acids synthesized in the cancer cells through de novo lipogenesis is important for the cellular membrane synthesis for proliferation, modulation of FAS to control the lipogenesis is a potential therapeutic target for anti-cancer drug candidates. To study the drug's efficacy and its mechanism of action against FAS, catalytically active and pure FAS is required. The commercially available FAS may be pure but it is not active thus not appropriate for an activity assay. And the conventionally used crude lysates for a typical enzymatic activity studies lack purity. We have purified FAS from MCF-7 breast cancer and LNCaP prostate cancer cell lines using a method of precipitation, filtration, and using a magnetic particle. Furthermore, in an attempt to discover active compounds against FAS from natural products, we have evaluated the extracts of Glechoma Hederacea L. and Aster Glehni F. Schmidt, natural products known to have lipolysis and antiadipogenic activities, for their capability of inhibiting FAS.

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Z α domain of ADAR1 prefers to bind to Z-RNA better than Z-DNA

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Double-stranded RNA deaminase I (ADAR1) deaminates adenine in pre-mRNA to yield inosine (I), which codes as a guanine residue in mRNA. These A-to-I conversions can lead to functional changes in the resulting proteins. At its NH₂-terminus, ADAR1 has two left-handed Z-DNA binding domains and preferentially binds Z-DNA, rather than B-DNA, with high binding affinity. The main difference between DNA and RNA is the presence of the ribose 2'-OH groups; however, this difference makes the two macromolecules very different with regard to their biochemical behavior as well as the structures they adopt as double helices. Both B-DNA and A-RNA can undergo a transition to left-handed double-helical structures, referred to as Z-DNA and Z-RNA. The crystal structural study of the Z-DNA binding domain of ADAR1 complexed to a r(CG)₃ duplex RNA found that the Z-RNA helix is associated with a unique solvent pattern that distinguishes it from the otherwise similar conformation of Z-DNA. In order to characterize the molecular recognition of Z-RNA by ADAR1, we performed NMR experiments with complexes of ADAR1 bound to r(CG)₃ and these results were compared with those of Z-DNA, d(CG)₃, induced by ADAR1 previously reported. We compared to the binding affinity of Z α ADAR1 for both A-DNA and Z-DNA and characterized its A-Z transition activity.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-280**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

NMR dynamics study of SP-isoform from *Zoarces elongates Kner*

Seo-Ree Choi, Joon-Hwa Lee^{*}, Ae-Ree Lee, Yeo-Jin Seo

Department of Chemistry, Gyeongsang National University, Korea

Antifreeze proteins (AFPs) are found in a variety of cold-adapted (psychrophilic) organisms to promote survival at subzero temperatures by binding to ice crystals and decreasing the freezing temperature of body fluids. One of most widely studied classes of AFPs is the type III from arctic fish such as the ocean pout and Japanese notched-fin eel pout. The type III AFPs are small globular proteins that consist of one α -helix, three 3_{10} -helices, and two β -strands. The type III AFPs have been categorized into two subgroups, quaternary-amino-ethyl (QAE) and sulfopropyl-Sephadex-binding (SP), based on differences in their isoelectric points. The QAE isoforms is able to halt the growth of ice, whereas the SP isoforms are unable to stop the growth of ice crystals. In this study, we have investigated backbone dynamics analyses of two kinds of type III AFPs from Japanese notched-fin eel pout (*Zoarces elongates Kner*), nfeAFP6 (SP), nfeAFP6_tri at various temperatures. We also characterized the structural/dynamic properties of the ice-binding surfaces by analyzing the temperature gradient of the amide proton chemical shift and its correlation with chemical shift deviation from random coil. This study provides insight into the molecular basis of ice-binding and antifreezing activities of type III AFP isoforms.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-281**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Chemical Biology Tools for the Sphingosine-1-phosphate (S1P) metabolism

Hoyoung Jung, Ji Young Ahn¹, Jung-Min Kee^{*}

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Generally, phospholipids were regarded as the major components of membrane and products of simple biosynthetic events. Beyond its passive role, metabolites of sphingolipids have recently been found to play key roles in cell signaling. For example, sphingosine-1-phosphate (S1P) is known to regulate various crucial physiological events such as angiogenesis, proliferation, and autophagy. As a result, phospholipid kinases have been regarded as promising drug targets for cancer, neurodegenerative diseases, and immune diseases. By the action of sphingosine kinase, S1P phosphatases and S1P lyase, the balance among S1P metabolites would be kept. However, it still remains elusive how the balance of these sphingolipids is dynamically regulated in vivo. Despite its biological importance, current research tools for monitoring lipid metabolism are laborious and indirect. Most of the methods rely on radioactive labeling, extraction and chromatography for identification and quantification. Consequentially, real-time measurements S1P metabolism are essentially impossible. To address these points, we herein report our progress in the development of fluorogenic chemical probes to investigate the complex metabolism and interconversion of signaling sphingolipids. Our probe design should also be applicable to the phosphorylation probes for other signaling lipids such as ceramides and diacylglycerols. These tools will enable high-throughput screening of the activators/inhibitors of enzymes. Furthermore, monitoring of the enzyme reactivity in the living cell will provide invaluable biological insights for understanding the lipid signaling pathways.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Thermal hysteresis activities of active and inactive isoforms of a type III antifreeze protein from Notched-fin eelpout, *Zoarces elongatus* Kner

Yeo-Jin Seo, Joon-Hwa Lee^{*}, Ae-Ree Lee, Seo-Ree Choi

Department of Chemistry, Gyeongsang National University, Korea

Antifreeze proteins (AFPs) or ice structuring proteins (ISPs) refer to a class of polypeptides produced by certain vertebrates, plants, fungi and bacteria that permit their survival in subzero environments. Type III antifreeze protein (AFP) is produced by several species of marine fishes (eelpouts) that inhabit ice-laden waters. The Japanese notched-fin eelpout, *Zoarces elongatus* Kner, produces 13 different AFPIII isoforms (denoted nfeAFP), which have been divided into six SP (nfeAFP1–6) and seven QAE (nfeAFP7–13) isoforms, and the latter was further divided into QAE1 (nfeAFP7–10) and QAE2 (nfeAFP11–13) isoforms. AFPs create a difference between the melting point and freezing point known as thermal hysteresis. The addition of AFPs at the interface between solid ice and liquid water inhibits the thermodynamically favored growth of the ice crystal. Ice growth is kinetically inhibited by the AFPs covering the water-accessible surfaces of ice. Thermal hysteresis is easily measured in the lab with a nanolitre osmometer. Organisms differ in their values of thermal hysteresis. QAE1 isoforms are fully active variants exhibiting both TH and ice-shaping activities but SP- and QAE2-isoforms are defective activity variants. In this study, we have performed thermal hysteresis activity analyses of six kinds of type III AFPs from *Zoarces elongatus* Kner, nfeAFP8 (QAE1), nfeAFP11 (QAE1), nfeAFP6 (SP), nfeAFP8_tri (Q9V/ L19V/ V20G), nfeAFP11_tri (V9Q/ V19L/ G20V) and nfeAFP6_tri (P19L/ A20V/ G42S). Our results provide insight into the molecular basis of ice-binding and antifreezing activities of type III AFP isoforms.

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Area: Life Chemistry

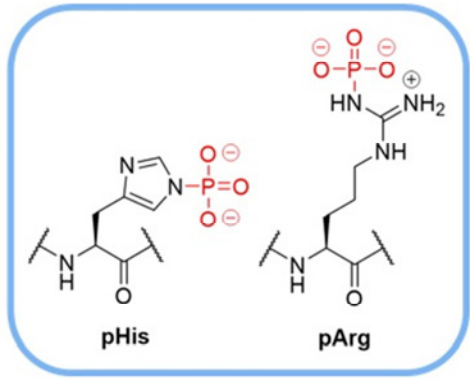
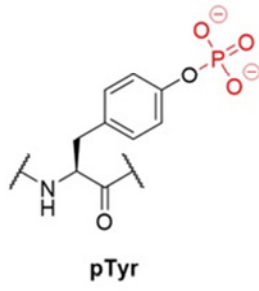
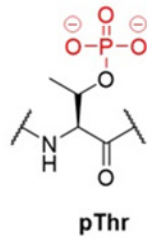
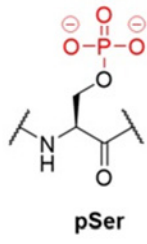
Type: Poster Presentation, Time: THU 11:00~12:30

Chemosensors for Protein N-Phosphorylations

Yigun Choi, Hoyoung Jung, Son Hye Shin, Jung-Min Kee *

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Protein phosphorylation controls the target protein functions, and it plays an important role in cell signaling and other physiological processes. Accordingly, misregulated phosphorylation has been linked to various human diseases including inflammation, diabetes, and cancer. In recent years, serine (Ser), threonine (Thr), and tyrosine (Tyr) phosphorylation have been studied extensively thanks to the advances in phosphoproteomics and other research tools. However, protein N-phosphorylations on histidine (His) and arginine (Arg) residues have been relatively unexplored because of their chemical instability and technical difficulties. Nonetheless, some important functions of these unconventional protein phosphorylations have been identified. For example, histidine phosphorylation is the key event in two component signal transduction systems, the major sensor systems in bacteria, plants, and fungi. And arginine phosphorylation regulates protein degradation and stress responses. Here, we report our progress in the development of fluorescence-based chemosensors for protein His/Arg phosphorylation. These chemosensors can be applied to real-time measurement of the kinase and phosphatase activities, with potential applications in high-throughput screening of the enzyme inhibitors/activators and discovery of novel His/Arg kinases.



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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Maleic acid amide derivatives for potential pH-sensitive drug release

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In drug delivery system, a variety of external stimuli, such as pH, redox potential, light, temperature, are exploited for controlled release of drug molecules. Among them, pH is one of the most frequently used signals because pH varies widely at the organ, tissue, and even subcellular levels. In our group, pH-sensitivity of maleic acid amide derivatives has been studied. Maleic acid amide moieties contain cis double bond and it was shown that pH-sensitive degradability of maleic acid amide derivatives can be tuned by adjusting α , β -substituents. Also, pH and light dual sensitivity was achieved by introducing fumaric acid amide derivatives, trans isomers of maleic acid amide derivatives. Fumaric acid amide derivatives themselves are not degradable at acidic pH. However, they can be converted into corresponding cis isomer maleic acid amide derivatives under UV irradiation. Furthermore, a pH-sensitive drug carrier based on β -cyclodextrin (β -CD) and 1-methyl-2-(2'-carboxyethyl) maleic anhydrides (MCM) was developed. β -CD-MCM was conjugated with cephadrine (CP) with high efficiency and more than 80% of conjugated CP molecules could be released again at pH 5.5 within 30 minutes. In 2013, Radosz group reported that succinic acid amide bond, which is known to be stable under acidic condition, with adjacent guanidine groups can be decomposed at pH 5.0. Inspired by this report, effect of nearby guanidine groups on pH-sensitive degradability of succinic- or maleic acid amide bond is being studied in our lab.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-285**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Structure basis of SAM-dependent methyl transfer reaction catalyzed by enzyme, YrrM

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Transfer RNAs (tRNAs) that have proximately 100 nucleotides and 'clover leaf' structure play vital role in process of protein synthesis by ribosome. Post-transcriptional modification of RNA affects codon base-pairings and stable folding of tRNA among many types of organism. However, many RNA modification enzymes remain unknown and understanding of the combination between proteins and RNA is limited to the field of RNA modification. Here, we describe the structure and biochemical characterization of YrrM expressed in *Escherichia coli*, methyltransferase(MTase) family. S-Adenosyl-L-methionine(SAM)-dependent methyltransferases (MTases) are associated with a widely various biological processes including methylation of nucleic acids, proteins, and small molecules using common methyl donor, SAM. The three dimensional structure of Yrrm has been revealed by X-ray crystallography. Finally, we experimentally show enzymatic features of this methyl transfer reaction by in vitro assay.

Conference Date: October 18~20, 2017

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Code: **BIO.P-286**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Structural biochemistry of MccS and MccB in CxSAM-dependent production of a peptide antibiotic in *Bacillus amyloliquefaciens*

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Microcin C (McC) is a 'Trojan horse' peptide antibiotic, encoded by six-gene *mcc* cluster in some strains of *E. coli*. Biosynthesis of McC initiates with the MccB-directed adenylation on the C-terminal asparagine of MccA, a heptapeptide precursor (MRTGNAN). Once mature McC is exported from producing cells and taken up by other sensitive cells, proteolysis results in the release of the non-peptide moiety, causing the inhibition of aspartyl-tRNA synthetase activity. A simpler form of *mcc* gene cluster was identified in *Bacillus amyloliquefaciens*, which consists of four genes. Unlike in *E. coli*, the N-terminal domain of MccB attaches cytosine at the C-terminal asparagine of MccA and the C-terminal domain of the MccB additionally modify cytosine moiety by carboxymethylation. *B. amyloliquefaciens* MccS, a homologue of *E. coli*, CmoA, synthesizes carboxy-S-adenosyl-L-methionine (cxSAM) which is the substrate of carboxymethylation, which inactivates the mechanism of resistance to McC in the sensitive cell. Here we present the X-ray crystal structure of MccS, demonstrating the structural diversity from that of *E. coli* CmoA. In addition, we have analyzed the in vitro activity of bifunctional MccB, the second instance of the use of CxSAM in living cells. Our studies support the hypothesis that biological use of CxSAM may be widespread, not just confined in tRNA modification.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-287**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Structural and functional characterization of a wobble uridine modifying enzyme from *Mycobacterium tuberculosis*

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To date, ~140 modified nucleosides have been identified in RNA, where most of them are observed among tRNA. These post-transcriptional modifications are formed via enzymatic reactions, and the list of such RNA modifying activity is still expanding. Recently, our laboratory has discovered a novel O-methyl transferase, YrrM, acting on tRNA in *Bacillus subtilis*. The enzyme directs the methylation of hypomodified wobble uridine (5-hydroxyuridine) on several isoacceptors in Gram-positive bacteria. The homologous search led us to identify a candidate enzyme from MTB, which shares ~38% (CHECK!) sequence identity with *B. subtilis* YrrM. Here we present the X-ray crystal structure and in vitro data of the MTB O-methyltransferase, supporting its role in tRNA modification.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **BIO.P-288**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Heteroaromatic Sulfones: New Chemical Tools for Selective Detection of Biothiols

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In biological studies, the selective reaction of chemical reagents with protein thiols is very important. This chemical reaction is employed to prevent cysteine-based cross-linking of proteins in common proteomics workflows. In addition, it is applied widely in targeted redox investigations of the mechanisms for understanding physiological and pathological processes in living systems. However, commonly used thiol blocking reagents like iodoacetamide (IAM), N-ethylmaleimide, and others were found to react with protein sulfenic acids (RSOH) which results in many significant errors in biological research. In this presentation, we will report a new heteroaromatic alkylsulfone, 4-(5-methanesulfonyl-[1,2,3,4]tetrazol-1-yl)-phenol (MSTP), as a selective and highly reactive biothiol blocking reagent for biological applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facile Synthesis of Fluorescent Labeled Peptides by Cysteine-Citrate Based Ring Formation

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Division of Chemistry, Seoul National University, Korea

Fluorescent labeling has been used as an important tool for detection of functional molecules in the biological system. Various fluorescent substances have been studied, however, limited biocompatibility and relatively high cost of fluorescent substances still need improvement for the application in biosystem. Therefore, it is important to develop fluorescent labeling method for simple and low-cost. In a previous research, it was reported that 5-oxo-2,3-dihydro-5H-[1,3]thiazolo[3,2-a]pyridine-3,7-dicarboxylic acid (TPA), a blue fluorescent substance with a high-quantum yield, could be synthesized from citrate and cysteine via one-step reaction. It is very promising for the biocompatible and low-cost fluorescent substance because both citrate and cysteine are highly-biocompatible and common substances in biological systems. However, the reaction has low yield and very high-temperature condition around 150 °C, which is difficult to be applied for the direct labeling onto the biological samples such as proteins or peptides. Therefore, in this study, inspired by the fact that TPA is formed from citrate and cysteine through two amide bonds, we developed a new method for simultaneous TPA formation and direct TPA labeling onto peptides in mild reaction conditions that could be applied to typical solid phase peptide synthesis (SPPS). TPA can be synthesized from citrate and cysteine in presence of a peptide-coupling reagent, which is confirmed by NMR and MS. The synthetic yield is greatly enhanced by the coupling reagent even at low temperature. Moreover, citrate treatment can form a TPA-labeled peptide from a cysteine-terminated peptide on the SPPS resin in the same reaction condition. Finally, we observed the blue fluorescence of the TPA-labeled peptide inside HeLa cells.

Conference Date: October 18~20, 2017

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Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Phase Determination of Iron-Dependent Homogentisate Dioxygenase from *Acinetobacter oleivorans*

Suk-Youl Park^{*}, Seung-A Hwangbo

Structural Biology Group, Pohang Accelerator Laboratory, Korea

In aromatic compounds mineralizing bacterium *Acinetobacter oleivorans*, homogentisate 1,2-dioxygenase (aoHGO) catalyzes the conversion of homogentisate to 4-maleylacetoacetate by aromatic ring scission using zinc ions, in the breakdown of tyrosine and phenylalanine. To determine the molecular background of the enzymatic mechanism of HGO in this iron-resistant organism, DH17_10945 encoding aoHGO of *Acinetobacter oleivorans* was cloned, and the expressed protein was purified. The protein was crystallized in 0.2 M sodium chloride, 25% [w/v] polyethylene glycol 3350 and 0.1 M BIS-TRIS at pH 6.5. X-ray diffraction data were collected to 1.5 Å resolution using synchrotron radiation. The crystal belongs to the orthorhombic space group C2221, with unit cell dimensions of $a = 53.1 \text{ \AA}$, $b = 121.2 \text{ \AA}$, and $c = 54.4 \text{ \AA}$. A traceable electron density map was calculated using anomalous diffraction data obtained from a crystal soaked in zinc ions.

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Code: **BIO.P-291**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The Arg/N-end rule pathway as positive regulator of autophagic flux & proteotoxic protein degradation

JEEYOUNG LEE, Won Hoon Choi, Min Jae Lee*

College of Medicine, Biochemistry, Seoul National University, Korea

The N-terminal amino acid of a protein is an essential determinant of ubiquitination and subsequent proteasomal degradation in the N-end rule pathway. We show here that blocking the arginylation branch of the pathway (Arg/N-end rule pathway) significantly impaired the fusion of autophagosomes with lysosomes by using para-chloroamphetamine (PCA) as a specific inhibitor of the Arg/N-end rule pathway. Under ER stress, the N-terminal arginylation of the ER heat shock protein HSPA5 (HSPA5/GRP78/BiP) that originally targets cargo proteins is moved out by ATE1-encoded Arg-tRNA-protein transferases in the cytosol, along with p62, to the autophagosome. At the late step of autophagy, proteasomal degradation of N-terminally arginylated HSPA5 (Arg-HSPA5) could role as a critical checkpoint for the proper progression of autophagic flux in the cells. Cells continuously treated with PCA exhibited increased levels and aggregation of autophagic markers such as LC3, p62, and proteotoxic proteins like tau and huntingtin. Treatment the Arg/N-end rule inhibitor in cells enhanced proteotoxic stress-induced cytotoxicity. Quantitative mass spectrometry with stable isotope labeling by amino acids in cell culture (SILAC) revealed that PCA significantly makes some changes in various biological pathways such as primarily cellular responses to stress, autophagic responses. Thus, the Arg/N-end rule pathway may actively protect cells from the negative influence of accumulated toxic proteins under various stress conditions. The Arg/N-end rule pathway has the first regulatory function in autophagy for substrate selection and the UPS-mediated degradation of Arg-HSPA5 helps the fusion of autolysosomes. Therefore, the Arg/N-end rule pathway may play a significant role of positively regulating autophagic flux under a number of stress conditions for protecting cells from harmful influences of proteotoxic protein accumulation.

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Code: **BIO.P-292**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Docosahexaenoic acid-mediated protein aggregates may reduce proteasome activity and delay myotube degradation during muscle atrophy *in vitro*

Ji Hyeon Kim, Do Hoon Park, Min Jae Lee*

College of Medicine, Biochemistry, Korea

Proteasomes are the degradation machinery for oxidatively damaged proteins including misfolded protein substrates. Cellular levels of reactive oxygen species increase with age and this cellular propensity is particularly harmful when combined with the age-associated development of various human disorders. Proteasome activity is reportedly downregulated in these disease conditions. Herein, we report that docosahexaenoic acid (DHA), a major dietary omega-3 polyunsaturated fatty acid, mediates protein aggregates through oxidation which reduce proteasomal activity. Cellular models overexpressing tau showed significantly elevated levels of aggregates and total ubiquitin conjugates in the presence of DHA, thereby reflecting suppressed proteasome activity. Strong synergetic cytotoxicity was observed when the cells overexpressing tau were simultaneously treated with DHA. Antioxidant N-acetyl cysteine significantly desensitized the cells to DHA-induced oxidative stress. DHA significantly delayed the proteasomal degradation of muscle proteins in a cellular atrophy model. Thus, the results of our study identified DHA as a potent inducer of cellular protein aggregates that inhibit proteasome activity and potentially delay systemic muscle protein degradation in certain pathologic conditions.

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Code: **BIO.P-293**

Area: Life Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Regulation of cellular proteasomal activity and autophagic flux via USP14 deubiquitinase

Kim Eunkyong, Seoyoung Park¹, Min Jae Lee^{*}

College of Medicine, Biochemistry, Seoul National University, Korea

¹*Department of Biochemistry and Molecular Biology, Seoul National University College of Medicine, Korea*

Two major intracellular pathways regulating protein degradation are the ubiquitin-proteasome system (UPS) and the autophagy-lysosome system (autophagy). Several biochemical mechanisms underlying the possible complementary relation between two of them have been suggested, however, little is known about the effect of enhanced proteasome activity on autophagic flux and its proteostatic consequences. Here, we found that activation of the proteasome through chemical and genetic inhibition of USP14, a proteasome-associated deubiquitinating enzyme, results in downregulation of autophagic flux in the cell. This autophagic impairment resulted mainly from delayed autophagosome-lysosome fusion and from abnormal turnover of UVRAG, a tumor suppressor and autophagic maturation regulator. Moreover, while proteasome activation through USP14 inhibition facilitated the clearance of a proteotoxic protein Tau and reduced the amount of its oligomeric forms, the same conditions increased formation of inclusion bodies from non-proteasomal substrates such as huntingtin with long polyglutamine repeats. Taken together, our results suggested that USP14 may function as a common denominator in the compensatory negative feedback relation between the two major proteolytic processes in the cell. This biochemical connection may underline a more precise therapeutic strategy for various pathological conditions due to impaired UPS or autophagy.

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Code: ORGN.P-235

Area: Organic Chemistry

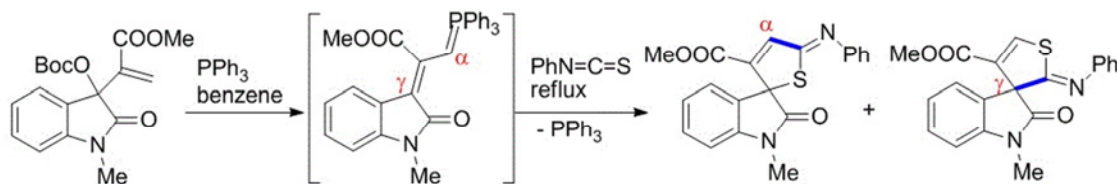
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Spirooxindoles Bearing Iminothiolactone Moiety from Morita-Baylis-Hillman Carbonates of Isatins and Phenyl Isothiocyanate

Beom Kyu Min, Da Young Seo, Hwa Jung Roh, Jae Nyoun Kim *

Department of Chemistry, Chonnam National University, Korea

Various spirooxindoles bearing iminothiolactone and thiolactone moieties have been synthesized by the reaction of MBH carbonates and isothiocyanates in the presence of PPh₃ in moderate to good yields.



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Code: **ORGN.P-236**

Area: Organic Chemistry

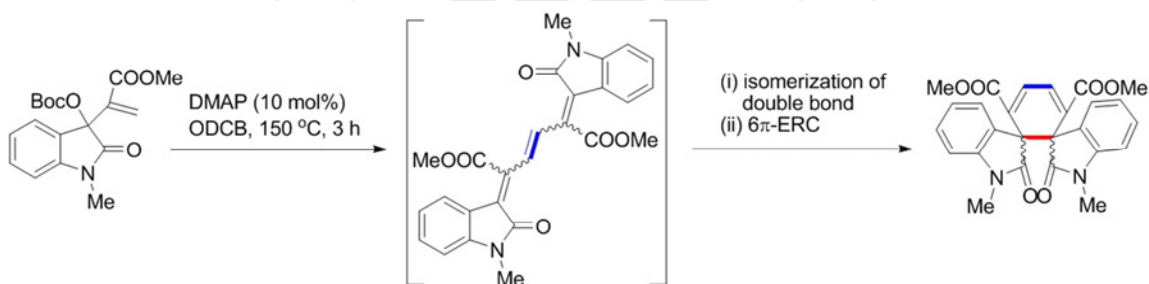
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Dispirocyclohexadiene Bisoxindoles from Morita-Baylis-Hillman Carbonates of Isatins

Beom Kyu Min, Hwa Jung Roh, Da Young Seo, Jae Nyoung Kim*

Department of Chemistry, Chonnam National University, Korea

6 π -Electrocyclization of trienes derived *in-situ* from the Morita-Baylis-Hillman carbonates of *N*-methylisatins afforded dispirocyclohexadiene bisoxindoles in good yields. Two stereoisomers (*cis* and *trans*) were formed in almost equal amounts.



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Area: Organic Chemistry

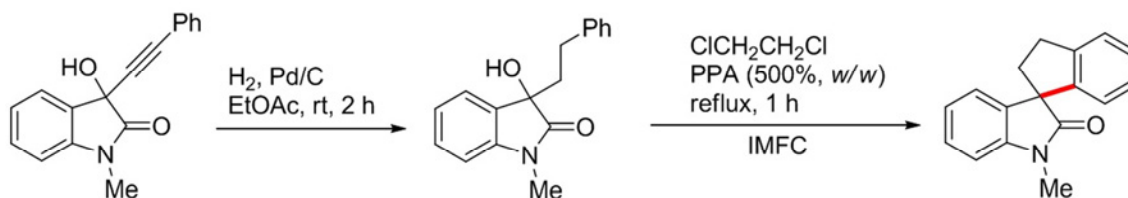
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Spiroindanyl-2-oxindoles via PPA-Mediated Intramolecular Friedel-Crafts Reaction

Da Young Seo, Hwa Jung Roh, Beom Kyu Min, Jae Nyoung Kim*

Department of Chemistry, Chonnam National University, Korea

Various spiroindanyl-2-oxindoles have been synthesized via PPA-mediated intramolecular Friedel-Crafts reaction of 3-arylethyl-2-oxindoles. 3-Arylethyl-2-oxindoles were prepared by catalytic hydrogenation of the propargylic alcohols derived from *N*-methylisatins.



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Area: Organic Chemistry

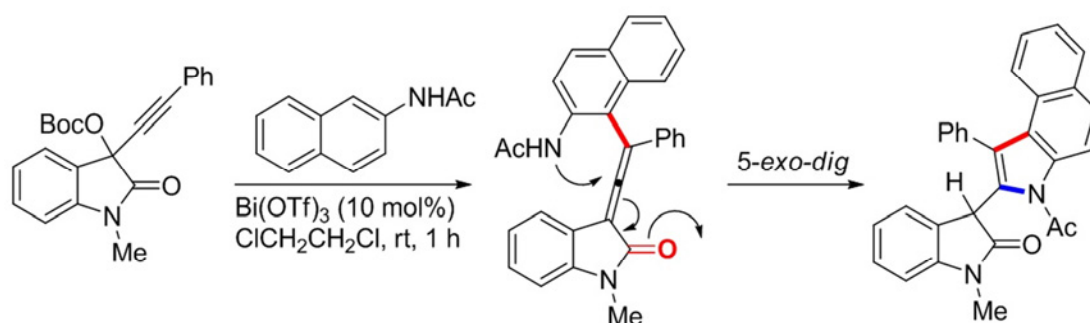
Type: Poster Presentation, Time: FRI 13:00~14:30

One-Pot Synthesis of 3-(Benzo[e]indol-2-yl)-2-oxindoles from Isatin-derived Propargylic Alcohols and *N*-Acetyl-2-aminonaphthalenes

Hwa Jung Roh, Da Young Seo, Beom Kyu Min, Jae Nyoung Kim*

Department of Chemistry, Chonnam National University, Korea

Various 3-(benzo[e]indol-2-yl)-2-oxindoles were synthesized by the reaction of isatin-derived propargylic alcohol derivatives and *N*-acetyl-2-aminonaphthalenes via Friedel-Crafts allenylation and Michael type 5-*exo-dig* cyclization.



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Area: Organic Chemistry

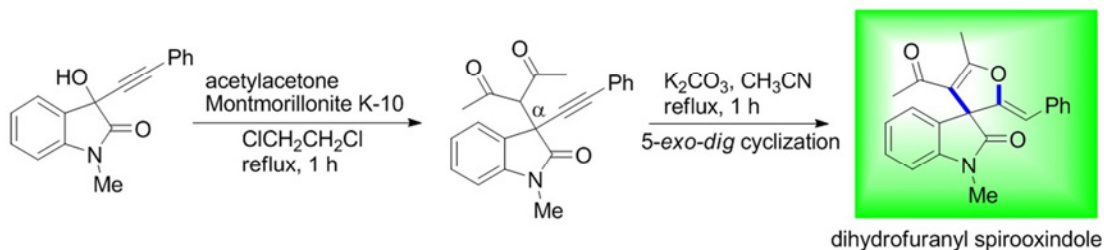
Type: Poster Presentation, Time: FRI 13:00~14:30

An Efficient Synthesis of Dihydrofuranyl Spirooxindoles from Isatin-Derived Propargylic Alcohols and 1,3-Dicarbonyls

Hwa Jung Roh, Beom Kyu Min, Da Young Seo, Jae Nyoung Kim*

Department of Chemistry, Chonnam National University, Korea

Various dihydrofuranyl spirooxindoles have been synthesized via montmorillonite K-10-catalyzed propargylation of 1,3-dicarbonyl compounds with isatin-derived propargylic alcohols and subsequent base-mediated 5-*exo-dig* cyclization.



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Type: Poster Presentation, Time: FRI 13:00~14:30

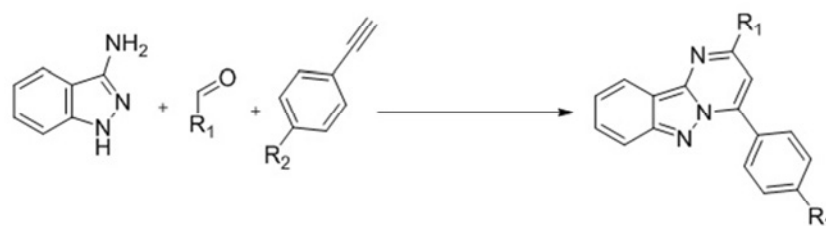
Green synthesis and characterization of silver nanoparticles (Ag NPs) from extract of plant Radix Puerariae: An efficient and recyclable catalyst for the construction of pyrimido[1,2-b]indazole derivatives under solvent-free conditions

SANDIP GANGADHAR BALWE, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

We have developed a green and environmentally friendly approach for the synthesis of silver nanoparticles (Ag NPs) using Radix Puerariae plant extract via a novel chemical route. The prepared Ag NPs has been characterized by TEM, XRD, SEM, DLS, EDX, and UV-Vis. Further, catalytic application of this fascinating nanomaterial has been utilized in the synthesis of pyrimido[1,2-b]indazole derivatives via one-pot three component coupling reaction under solvent-free conditions.

Scheme



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-241**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

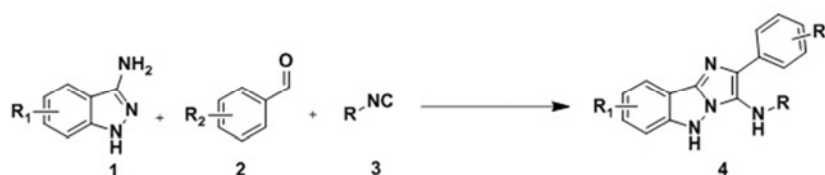
Synthesis of diverse nitrogen-enriched tricyclic novel (imidazo[1,2-b]indazol-3-amines) scaffolds using one-pot multicomponent reaction under mild reaction conditions

SANDIP GANGADHAR BALWE, Yeon Tae Jeong^{*}

Department of Display Engineering, Pukyong National University, Korea

A novel and expedient one-pot synthesis of (imidazo[1,2-b]indazol-3-amines) derivatives from 3-amino-1-H-indazole and aldehydes with isocyanide has been developed. This protocol features mild reaction conditions, robust method, one-step construction of privileged tricyclic rings, clean reaction profile, operational simplicity and tolerate a diverse collection of reactants.

Scheme



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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-242**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

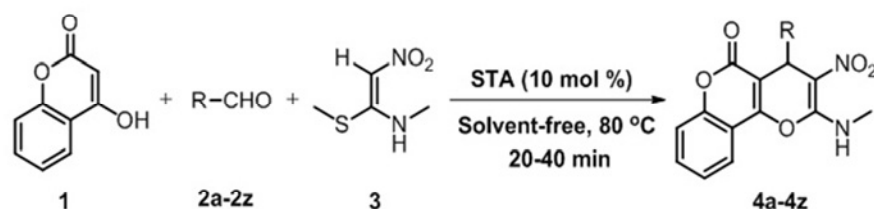
A highly efficient and recyclable silica-supported tungstic acid (STA) catalyst for the synthesis of pyrano[3,2-c]chromen-5-ones under solvent free conditions

amol jadhav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

Synthesis of pyrano[3,2-c]chromen-5-ones have been synthesized by an efficient, simple and green one-pot domino protocol by multi-component condensation of 4-hydroxycoumarin, aldehydes and (E)-N-methyl-1-(methylthio)-2-nitroethenamine in the presence of a catalytic amount of silica-supported tungstic acid (STA) under solvent-free conditions. The salient features of this protocol are simple reaction procedure, shorter reaction time, good yields, avoidance of aqueous work-up, and column chromatographic separation. The merit of this process is highlighted by its high bond efficiency of producing three new bonds and one stereocenter in a single operation.

Scheme



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

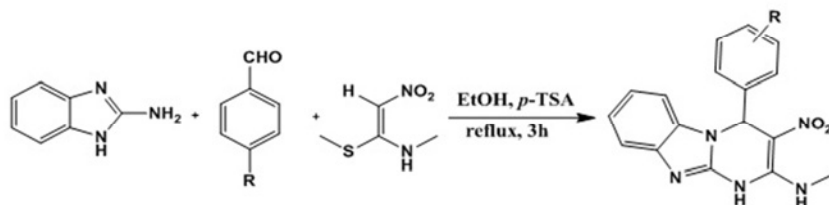
An efficient one-pot three-component synthesis of N-methyl-3-nitro-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidin-2-amine derivatives using p-TSA as catalyst

amol jadhav, Yeon Tae Jeong^{*}

Department of Display Engineering, Pukyong National University, Korea

A simple, efficient, eco-friendly, and cost-effective method has been developed for the synthesis of N-methyl-3-nitro-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-a] pyrimidin-2-amine derivatives using 1H-benzo[d]imidazol-2-amine, aldehydes and (E)-N-methyl-1-(methylthio)-2-nitroethenamine, in the presence of catalytic amount of p-toluenesulfonic acid (p-TSA) in ethanol under reflux conditions. The advantages of this method are the use of an inexpensive and readily available catalyst, shorter reaction times, a wide range of functional group tolerance, and high yield of products via a simple experimental and work-up procedure.

Scheme



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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-244**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Dihydrophosphaisocoumarins through a Palladium-Catalyzed Oxidative Cyclization of Arylphosphonic Acid Monoethyl Esters with 1,3-Dienes

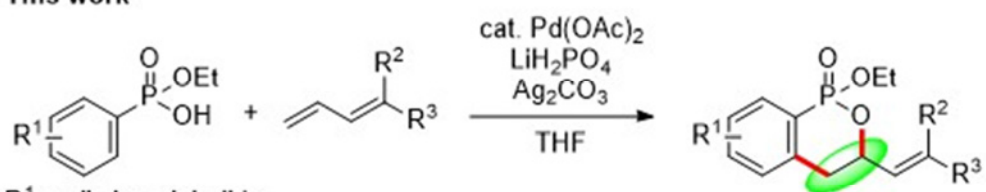
Kyusik Um, hyunseok kim¹, Phil Ho Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹*Kangwon National University, Korea*

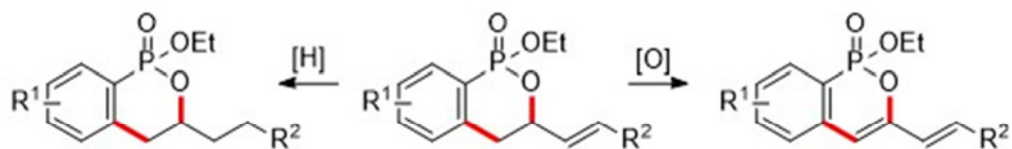
Organophosphorus compounds are an omnipresent structural motif found in living organisms and biologically active compounds, and their facile synthesis is important in the preparation of synthetic intermediates, agrochemicals, and pharmaceuticals. Additionally, these compounds have continuously attracted great interest due to their role as bioisosteres of carbonyl and carboxylate groups. Accordingly, much effort has been devoted not only to construct skeletons of phosphorus compounds but also to introduce new functional groups onto these compounds. However, in contrast their acyclic analogs, the synthesis and application of phosphaheterocyclic compounds have been rarely investigated. We developed an efficient synthetic method for the selective preparation of dihydro-phosphaisocoumarins and their derivatives through a Pd-catalyzed oxidative cyclization reaction of a wide range of arylphosphonic acid monoethyl esters with activated and unactivated 1,3-dienes, including 1-aryl-substituted 1,3-dienes and 1-alkyl-substituted 1,3-dienes, thus opening a new avenue for the synthesis of phosphaheterocyclic compounds.

This work



R¹ = alkyl, aryl, halide

R², R³ = alkyl, aryl, electron-withdrawing group



Wild substrate scope

Highly regioselective

Simple and readily available starting materials



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-245

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Cyclic Sulfoximines from Sulfoximines and 3-Diazoindolin-2-imines

Gi Hoon Ko, hyunseok kim¹, Kyusik Um, Phil Ho Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹Kangwon National University, Korea

Sulfoximines are significant compounds that are found in pharmaceuticals, bioactive compounds, and agrochemicals. Accordingly, the development of novel synthetic methods for sulfoximines and their modifications have become highly attractive. To date, many synthetic methods using these tools have been reported in the literature. These methods have focused mainly on the preparation of linear sulfoximines and their derivatives. However, synthetic approaches for the construction of cyclic sulfoximines have been relatively limited. We developed a novel synthetic method for indolo-1,2-benzothiazines via the Rh-catalyzed cyclization of *S*-aryl sulfoximines with 3-diazoindolin-2-imines together with the release of molecular nitrogen and *p*-toluenesulfonamide. The present method involved the N-H/C-H activation of *S*-aryl sulfoximines. A wide-ranging scope of both *S*-aryl sulfoximines and 3-diazoindolin-2-imines was demonstrated. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

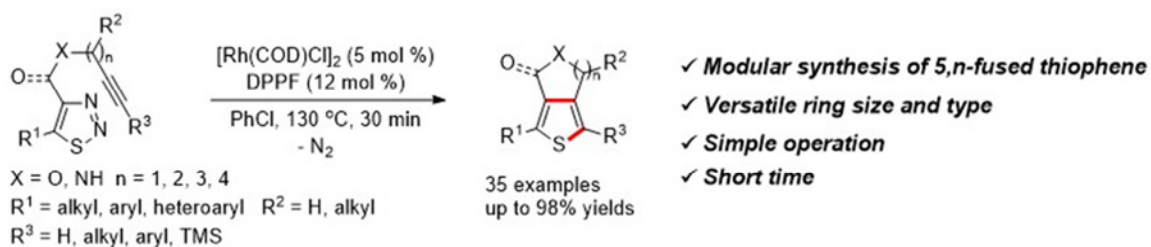
Rhodium-Catalyzed Intramolecular Transannulation of Alkynyl Thiadiazole

Younghyeon Baek, Da-Hye Jeon, Dongjin Kang¹, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

¹Department of Pharmaceutics, Inje University, Korea

Fused thiophenes have been recognized as very important scaffolds in the field of pharmaceutical and functional materials sciences. For this reason, the development of an efficient synthetic method for functionalized fused thiophenes is highly attractive and poses a significant challenge. However, because some of the previously reported synthetic methods demand a strong base, long reaction times, and vigorous reaction conditions, the development of efficient synthetic approaches to overcome these shortcomings has been continuously required. Herein, we developed a method for the synthesis of a wide range of fused thiophenes, including those fused with lactams, lactones, or cyclic ethers, from a rhodium-catalyzed intramolecular transannulation reaction of alkynyl thiadiazoles. This transannulation reaction provides an efficient platform for the construction of a variety of 5,n-fused thiophenes from readily available starting materials together with the release of molecular nitrogen.



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Area: Organic Chemistry

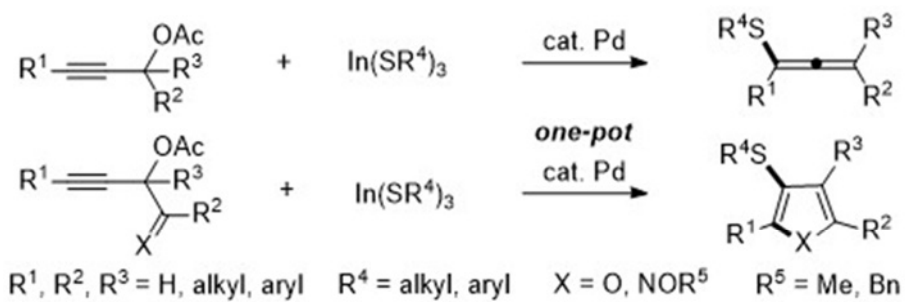
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Multisubstituted Allenes, Furans, and Pyrroles via Tandem Palladium-Catalyzed Substitution and Cycloisomerization

Da-Hye Jeon, Gi Hoon Ko, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Recently, an efficient synthetic method towards multisubstituted furans and pyrroles bearing hetero-substituents was reported through metal-catalyzed 1,2-shifts of diverse migrating groups in allenyl systems. However, the introduction of a wide variety of substituents at the 4-position of furans and pyrroles is impossible due to requirement of [1,3]-H shift in these methods. Therefore, the development of an efficient synthetic method for multisubstituted furans and pyrroles bearing 3-heteroatom substituents as well as substituents at the 4-position has been a continuing challenge. Herein, we report Pd-catalyzed propargyl substitution reactions of propargyl acetates with indium organothiolates for the synthesis of multisubstituted allenyl sulfides. This procedure employed tandem Pd-catalyzed propargyl substitution and cycloisomerization reactions from indium organothiolates and propargyl acetates bearing acyl and imidoyl groups for the synthesis of multisubstituted furans and pyrroles in one-pot. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



one-pot tandem reaction

Highly regioselective

Readily available starting materials



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Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-248

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Benzofulvene Derivatives via Rh-Catalyzed Transannulation of Enynyl Triazoles

Uiseong Yeon, Sang Hoon Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Benzofulvenes are key privileged scaffolds present in natural products, biologically and pharmacologically active molecules, functional materials, and metallocene catalysts. Due to its significance, it is still of considerable interest and necessity to develop efficient synthetic methods for functionalized benzofulvenes. Recently, *N*-sulfonyl-1,2,3-triazoles, easily obtained from click reactions, have been used for the preparation of a large number of heterocyclic and carbocyclic compounds through Rh-catalyzed denitrogenative cyclization. On the basis of these results, Rh-catalyzed denitrogenative cyclization of (*E*)-ethyl 2-(1-alkyl and arylsulfonyl-1*H*-1,2,3-triazol-4-yl)-3-aryl acrylate generated from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in the presence of a copper catalyst was demonstrated for the synthesis of a wide range of functionalized benzofulvenes. Additionally, we have developed straightforward synthetic procedures for three benzofulvenes through tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in a one-pot.



R¹ = H, 2-Me, 3-Me, 4-Me, 4-MeO, 3,5-(MeO)₂, 4-Cl, 3-Br, 4-AcO, 2-F-4-MeO

R¹-C₆H₄ = 2-naphthyl, 2-furyl

R² = Me, *i*-Pr, 4-Me-C₆H₄, 4-MeO-C₆H₄

X = CO₂Et, CH₂OMe, Ac

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-249**

Area: Organic Chemistry

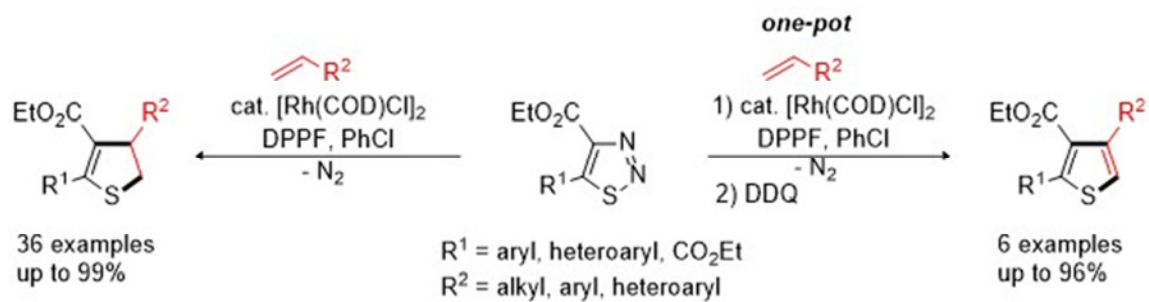
Type: Poster Presentation, Time: FRI 13:00~14:30

Regioselective Synthesis of Dihydrothiophenes and Thiophenes through the Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Alkenes

Jeong-Yu Son, Sang Hoon Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Sulfur-containing five-membered heterocyclic compounds such as dihydrothiophenes and thiophenes represent key structural motifs due to their biological activities in natural products and pharmaceuticals. In addition, thiophene derivatives are very attractive compounds in the field of material science due to their peculiar structural rigidity and useful electronic properties. Thus, the development of synthetic methods for these core scaffolds has received considerable attention in contemporary chemistry. The regioselective introduction of a wide range of substituents onto dihydrothiophene and thiophene rings from readily available starting materials is required. In this study, the regioselective synthesis of a wide range of dihydrothiophenes was developed from the rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with aliphatic, aromatic, and heteroaromatic alkenes. Tandem rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with alkenes followed by 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) oxidation was also demonstrated for the one-pot regioselective synthesis of various thiophenes. This method was employed to efficiently synthesize pentaoligomeric compounds consisting of three benzene and two dihydrothiophene rings. Advantages of the present method include a broad substrate scope, wide functional group compatibility, and high regioselectivity. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



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Code: **ORGN.P-250**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Isothiazoles through Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Nitriles

Boram Seo, kuhwan jeong, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Isothiazoles are valuable structural motifs found in many natural products, pharmaceutical compounds, and functional materials. For this reason, streamlined methods for their synthesis from readily available compounds must be developed. Herein, we developed a synthetic method for obtaining a wide variety of isothiazoles by the Rh-catalyzed transannulation of 1,2,3-thiadiazoles with alkyl, aryl, and heteroaryl nitriles, which proceeds via an α -thiavinyl Rh-carbenoid intermediate. The results suggest that during its reaction with nitriles, the α -thiavinyl carbene acts as an umpolung 1,3-dipole equivalent, in contrast to its behavior during its reaction with alkynes. The developed method was successfully employed to synthesize pentaoligomeric arylene compounds consisting of three benzene and two isothiazole rings.



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Code: **ORGN.P-251**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

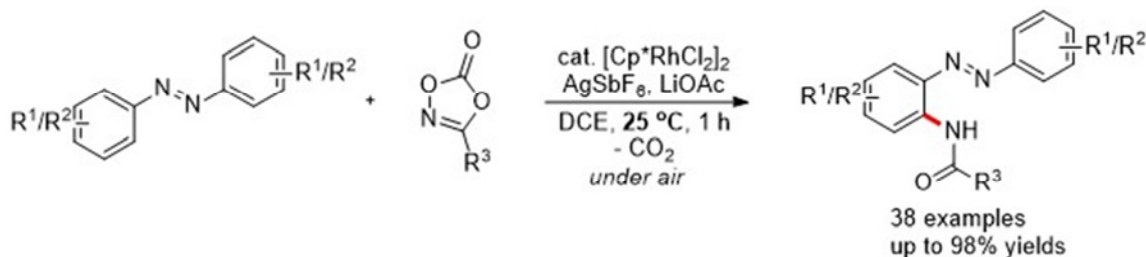
Selective Rhodium-Catalyzed C-H Amidation of Azobenzenes with Dioxazolones

Uiseong Yeon, kuhwan jeong, Dongjin Kang¹, Phil Ho Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹*Department of Pharmaceutics, Inje University, Korea*

Azobenzenes are a significant class of compounds in many fields, such as organic dyes, food additives, and material science. Thus, development of streamlined synthetic methods for their derivatives is greatly needed. Although the introduction of a wide range of functional groups onto a symmetrical azobenzene ring has been reported, selective introduction of substituents onto unsymmetrical azobenzenes still represents a formidable challenge. In our continuing efforts in C-H activation, we have been interested in the development of direct and selective C-N bond formation using both symmetrical and unsymmetrical azobenzenes under mild conditions. Herein, we present an efficient synthetic method for a wide range of amidated azobenzenes through the selective Rh-catalyzed C-H amidation reaction of symmetrical as well as unsymmetrical azobenzenes with alkyl-, aryl-, and heteroaryl-substituted dioxazolones under mild conditions. In addition, diamidation of azobenzenes and amidation of monoamidated azobenzenes will be presented.



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Area: Organic Chemistry

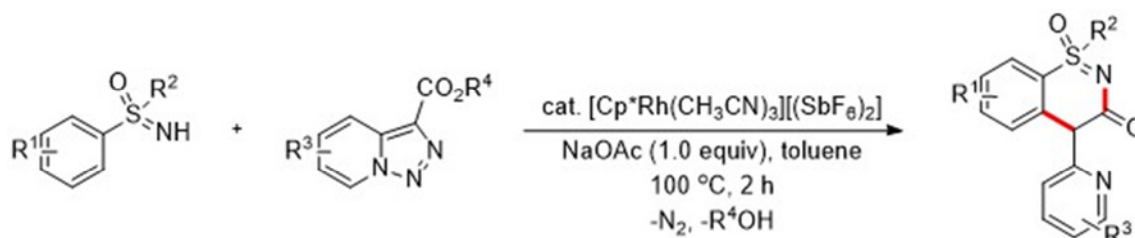
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of 1,2-Benzothiazines via a Rhodium-Catalyzed Cascade C-H Activation/Cyclization/Elimination Process from Sulfoximines and Pyridotriazoles

Jeong-Yu Son, Gi Uk Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Sulfoximines are novel privileged scaffolds that have been applied as pharmaceuticals and bioactive compound as well as ligands and chiral auxiliaries in asymmetric syntheses. As a consequence, the development of efficient methods for the synthesis of sulfoximines and their functionalizations is greatly needed. However, despite the significant advances made in the functionalization of sulfoximines, only a few examples of 1,2-benzothiazines, which are more attractive pharmacophores as a type of cyclic sulfoximine, have been reported. Herein, we have developed an efficient synthetic method for a wide range of 1,2-benzothiazines bearing pyridyl as well as carbonyl groups by a rhodium-catalyzed domino C-H activation/cyclization/elimination of alcohol process starting from *S*-aryl sulfoximine and pyridotriazole compounds. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



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Code: **ORGN.P-253**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

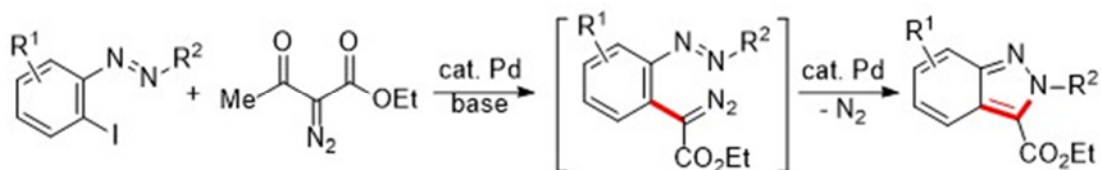
Synthesis of 2*H*-Indazoles via Palladium-Catalyzed Deacylative Cross-Coupling and Denitrogenative Cyclization from 2-Iodoazoarenes and 2-Iodoaryltriazenes

Gi Uk Han, Kyusik Um, Dongjin Kang¹, Phil Ho Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹*Department of Pharmaceutics, Inje University, Korea*

A synthetic method to prepare a wide range of 2*H*-indazoles was developed via a tandem Pd-catalyzed deacylative cross-coupling reaction of 2-iodoazoarenes and 2-iodoaryltriazenes with acyldiazoacetates and denitrogenative cyclization reaction of in situ generated diazoacetates having azoaryl and triazenyl aryl moieties in one-pot. Additionally, azoaryl-substituted diazoacetates underwent Pd-catalyzed denitrogenative cyclization to produce 2*H*-indazoles. The present reaction is a good example in which a Pd(0)-catalyst is involved in two catalytic cycles in one-pot. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

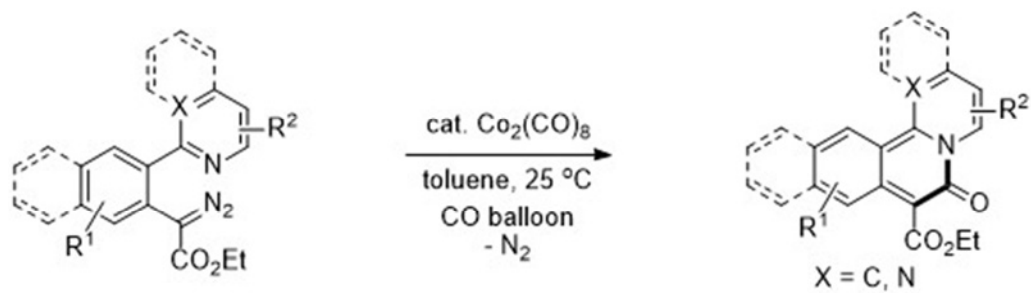
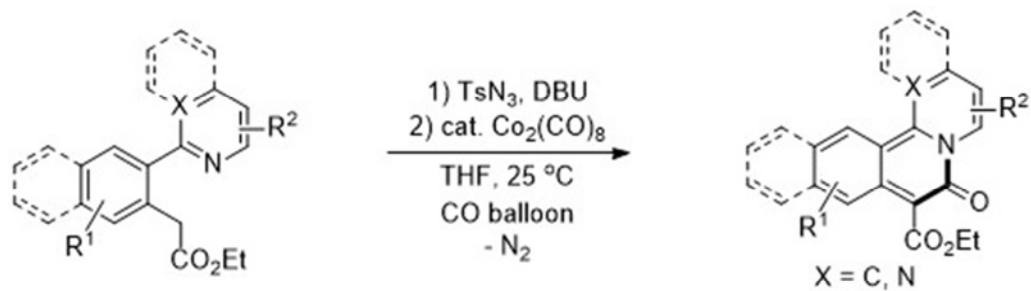
Synthetic Method of Pyridisoquinolinones via Cobalt-Catalyzed Carbonylative Cyclization of Pyridinyl Diazoacetates

Younghyeon Baek, Minhyeon Byeon, Dongjin Kang¹, Phil Ho Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹*Department of Pharmaceutics, Inje University, Korea*

Transition-metal-catalyzed carbonylation using carbon monoxide is one of the significant methods to prepare a variety of carbonyl compounds. In particular, Pd-catalyzed carbonylative cross-coupling is an important method for the synthesis of a large number of compounds having the carbonyl functional group. However, the carbonylation of metal carbenes is rarely reported due to the limitations of substrate scope and harsh conditions, such as the high pressure of carbon monoxide, high reaction temperature, and stoichiometric processes. Moreover, because the carbonylation of metal carbene furnishes ketenes, which are very important in organic synthesis, the development of streamlined synthetic methods to overcome these shortcomings is still highly attractive and challenging. In conclusion, we have successfully developed a dicobalt octacarbonyl catalyzed carbonylative cyclization of pyridinyl diazoacetates for the synthesis of pyridisoquinolinones under a carbon monoxide atmosphere. Moreover, a useful synthetic method for a wide range of pyridisoquinolinones from pyridinyl aryl acetates has been demonstrated through diazotization using TsN₃ and DBU followed by Co-catalyzed carbonylation and intramolecular cyclization of ketene with a tethering pyridinyl moiety under a carbon monoxide atmosphere in a semi-one-pot procedure. These transformations are attractive due to the use of an inexpensive and commercially available Co catalyst and an easily accessible starting material and the release of harmless N₂ under mild conditions (room temperature).



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Code: **ORGN.P-255**

Area: Organic Chemistry

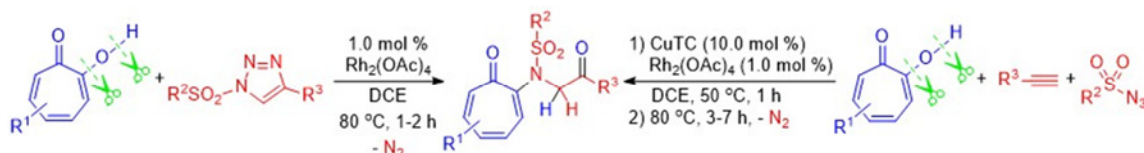
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of 2-Functionalized Tropones through Sequential Functionalization of O-H and C(sp²)-O Bonds of Tropolones

Boram Seo, Minhyeon Byeon, Phil Ho Lee *

Department of Chemistry, Kangwon National University, Korea

Tropolones make up a significant class of seven-membered non-benzenoid aromatic compounds that can be subjected to higher order cycloaddition reactions to provide a large number of biologically active compounds and natural products. Aminotroponimines derived from tropolone having a 2-hydroxy group are also a typical group of ligands. In this regard, introduction of new functional groups onto tropolone and transformation of previously present functional groups in the troponoid family are desirable. Although there are several methodologies for the preparation of functionalized tropolones in the literature, the development of new and convenient methods to prepare them is imperative. For this reason, we have developed the Rh-catalyzed reaction of tropolones with *N*-tosyl-1,2,3-triazoles for the synthesis of the 2-functionalized aminotropones via tandem Rh-catalyzed O-H insertion, intramolecular 1,8-addition, and rearrangement in one pot. Sequential Cu-catalyzed [3 + 2] cycloaddition, Rh-catalyzed O-H insertion, intramolecular 1,8-addition, and rearrangement starting from 1-alkynes, *N*-sulfonyl azides, and tropolones is also demonstrated for the synthesis of the 2-functionalized aminotropones in one pot. These results suggest that sequential functionalization of O-H and C(sp²)-O bonds smoothly take place in C(sp²)-O-H bonds at the 2-position of tropolone.



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Area: Organic Chemistry

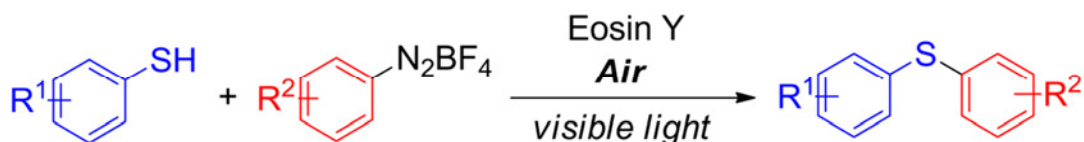
Type: Poster Presentation, Time: FRI 13:00~14:30

Visible-light-promoted synthesis of diaryl sulfides under air

Boseok Hong, Juyoung Lee, Anna Lee*

Department of Chemistry, Myongji University, Korea

Sulfur-containing organic molecules are of interest to scientists in several areas of research, from medicinal chemistry to material science. Among them, diaryl sulfides and their derivatives are important structural motifs in natural and synthetic molecules and have shown interesting biological and pharmaceutical activities. Moreover, they are precursors to other sulfur-containing compounds comprising higher-oxidation state-sulfur (sulfoxides, sulfones etc.), which have similar important bioactive properties. While previous synthetic methods have provided powerful tools for affording diaryl sulfides, still have some limitations such as sensitive/harsh reaction conditions or using prefunctionalized starting materials. Therefore, the development of novel and simple complementary strategies would be greatly valuable for the construction of C_{aryl}-S bonds. Herein, a broad range of aryl thiols reacted with various aryl diazonium salts in the presence of eosin Y under air atmosphere via visible-light mediated organocatalytic process. This novel and environmentally friendly method provides an alternative route to established synthetic approaches to afford the desired products from easily available substrates in high yields.



■ **organo-photocatalysis**

■ **air stable conditions**
: **open air**

■ **neutral pH / mild conditions**

■ **pretreated thiols**
: **not necessary**

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-257**

Area: Organic Chemistry

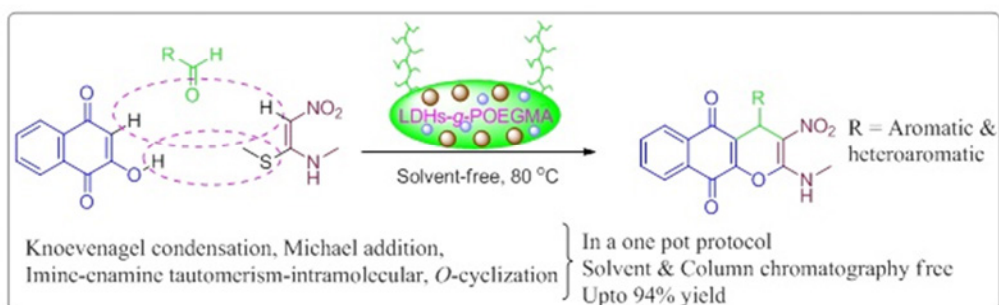
Type: Poster Presentation, Time: FRI 13:00~14:30

Solvent-free synthesis of 4H-pyranonaphthoquinones using highly active and stable polymer grafted layered double hydroxides (LDHs-g-POEGMA) as an efficient and reusable heterogeneous catalyst

KUMAR KRISHNAMMA, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

Benzo[g]chromene-5,10-diones (chromene-diones) have been synthesized by an efficient, simple and green one-pot domino protocol by multi-component condensation of 2-hydroxy-1,4-naphthoquinone with aldehydes and (E)-N-methyl-1-(methylthio)-2-nitroethenamine in the presence of poly(oligoethylene glycol methacrylate)-g-supported layered double hydroxides (LDHs-g-POEGMA), under solvent-free condition. The significant features of this “green” reaction include short reaction time, high product yields in pure form, eco-friendly method; avoid the toxic solvents and no need for purification of the product by column chromatography. Furthermore the catalyst (LDHs-g-POEGMA) is reused for several consecutive runs without losing its catalytic activity.



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Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-258

Area: Organic Chemistry

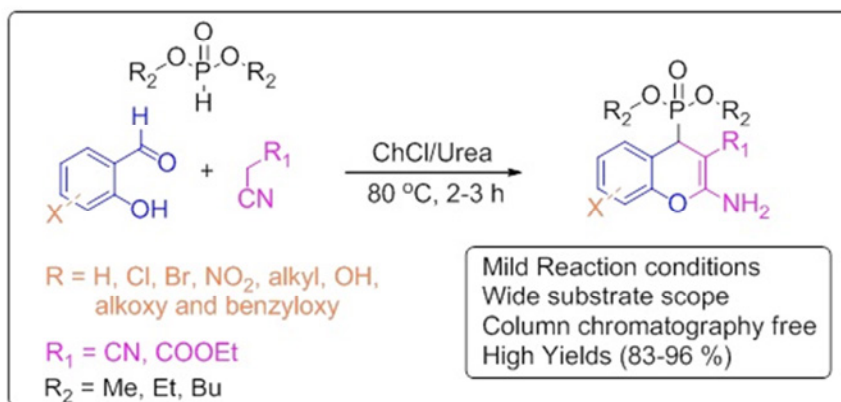
Type: Poster Presentation, Time: FRI 13:00~14:30

Choline chloride based deep eutectic solvent as an efficient solvent for the synthesis of 2-amino-3-cyano-4H-chromene-4-yl-phosphonate derivatives via multi-component reaction under mild and efficient conditions

KUMAR KRISHNAMMA, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

Synthesis of 2-amino-4H-chromen-4-ylphosphonates has been accomplished by the one-pot three-component reaction of salicylaldehyde, malononitrile/ethylcyanoacetate and dialkyl phosphites were carried out in the presence reusable deep eutectic solvent (DES) under mild conditions. The applicability of DES for the synthesis of 2-amino-4H-chromenes also has been described. The advantages of this methods is mild reaction conditions, simple work-up procedure, and use of DES as an inexpensive and green solvent provides an economical protocol for the preparation of important biological active phosphorus-containing compounds.



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Type: Poster Presentation, Time: FRI 13:00~14:30

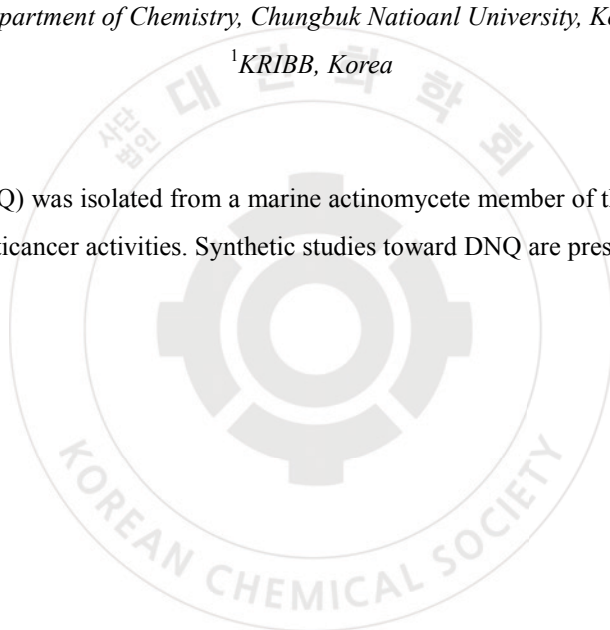
Synthetic Studies toward Deoxynboquinone

Jihee Yoon, Sangku Lee^{1,*}

Department of Chemistry, Chungbuk National University, Korea

¹*KRIBB, Korea*

Deoxynboquinone (DNQ) was isolated from a marine actinomycete member of the genus *Pseudonocardia*, and exhibited potent anticancer activities. Synthetic studies toward DNQ are presented.



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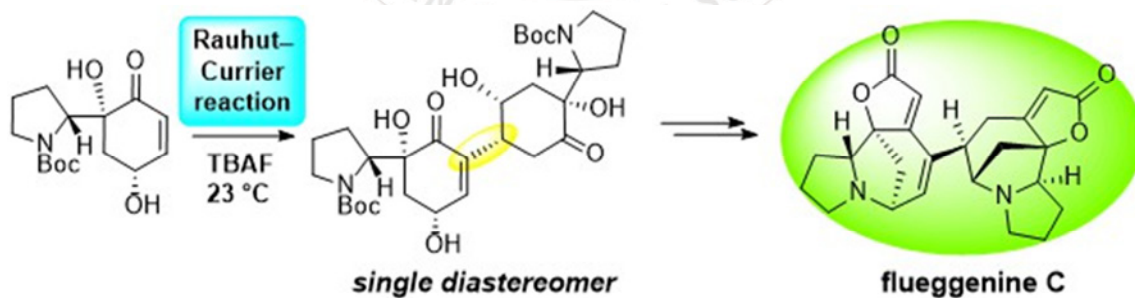
Type: Poster Presentation, Time: FRI 13:00~14:30

Total Synthesis of (-)-Flueggeine C via an Accelerated Intermolecular Rauhut–Currier Reaction

Sangbin Jeon, Sunkyu Han *

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

The first total synthesis of dimeric securinega alkaloid (-)-flueggeine C is completed via an accelerated intermolecular Rauhut–Currier (RC) reaction. Despite the numerous reports on the total synthesis of monomeric securinegas, the synthesis of dimeric securinegas whose monomeric units are connected by a putative enzymatic RC reaction has not been reported to date. We have found that an installation of a nucleophilic functional group at the γ -position of an enone greatly accelerates the rate of the diastereoselective intermolecular RC reaction. This discovery enabled an efficient and selective formation of the dimeric intermediate which was further transformed to (-)-flueggeine C.



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Venue: Kimdaejung Convention Center, Gwangju

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Derivatization of Peptoids Using Chan-Lam Reaction

Jihyun Song, Yong-Uk Kwon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Peptides are representative biomolecules that possess various physiological activities in vivo. Thus, they are attractive chemical tools for chemical biology and drug development. However, peptides have unwanted drawbacks including a proteolytic degradation, insufficient cell permeability, etc. To overcome these defects, many different types of peptidomimetics have been developed. Among them, peptoids emerged as valuable molecular tools. They have many advantages such as easy synthesis, tremendous diversity in library construction, resistance to proteolytic degradation and improved cell permeability. Hence, peptoids have attracted great attention to many chemists, pharmacologists, biologists, etc. The N-arylation/O-arylation methodology using Chan-Lam cross coupling reaction is a powerful synthetic tool. Therefore, we have employed Chan-Lam reaction in solid phase synthesis for efficient functionalization of peptoids to maximize their diversity. It was also applied to develop cyclic peptoids as a new macrocyclization method. In this presentation, we will report herein synthetic studies for the interesting derivatization of peptoids using Chan-Lam reaction on solid-phase.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Solid-Phase Total Synthesis of Peptoid-Based Daptomycin Analog

Hyun-Ju Im, Yong-Uk Kwon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Peptides are interesting molecules that can be used as chemical tools in medicine, biochemical sciences, protein capture and purification, diagnostics, etc. But, there are several unexpected drawbacks such as limited cell permeability, sensitivity to proteases and poor bioavailability. Therefore, various peptidomimetics have been developed to overcome these disadvantages. Among them, peptoids (N-substituted oligoglycines) not only complement these shortcomings but also have several advantages such as improved cell permeability, easy synthesis and high cellular stability. Especially cyclic peptoids may possess higher binding affinity against proteins because of increased conformational rigidity and relatively preorganized structures, compared to their linear counterparts. Moreover, if they have a specific site like lipid chain, they may be used as antibiotics based on their characteristics. Daptomycin is a molecule consisting of 10 amino acids in cyclic form and a linear 3 amino acid side chain modified with an undecanoyl lipid at the N-terminus. And it has potent bactericidal activity with a unique mode of action against otherwise antibiotic-resistant Gram-positive pathogens. Thus, we envisioned to develop peptoid-based daptomycin analog which might have better bioactivity than daptomycin and might also resolve resistance problems. In this presentation, we will introduce synthetic studies on new peptoid analog of daptomycin on solid-phase.

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Type: Poster Presentation, Time: FRI 13:00~14:30

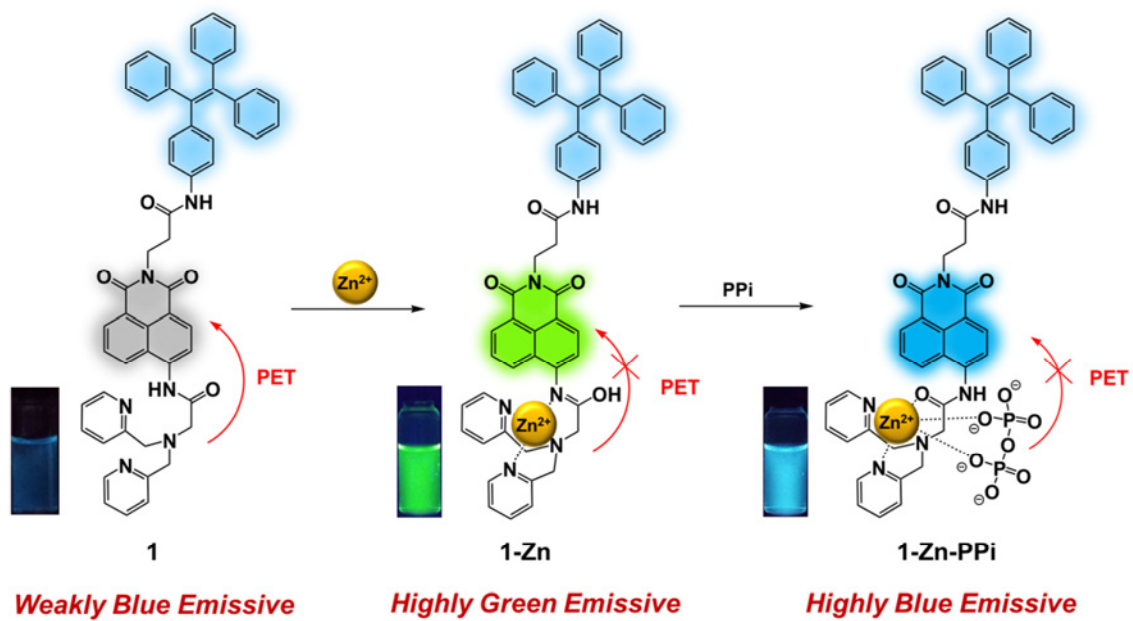
Highly selective dual-channel fluorescent probe for sensing of Zn²⁺ ions and pyrophosphate in micelle

Min Jung Chang, Min Hee Lee^{1,*}

Department of chemistry, Sookmyung Women's University, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Zn²⁺ is one of the significant cofactor in biological and pathological process such as brain function, gene transcription, immune function and Alzheimer's diseases. Along with this essential metal ion, pyrophosphate (P₂O₇⁴⁻, PPI) is also the most importantly biological involved anions in living systems. A lot of Zn²⁺-sensing and Zn²⁺ chelated PPI-sensing fluorescent probes have been developed. However, they suffered from poor limit of detection (LOD) and selectivity to Zn²⁺ and PPI, respectively. With this in mind, we reported a novel fluorescent probe 1, consists of naphthalimide as a fluorescence reporter, tetraphenylethene (TPE) as a well-known aggregation induced emission (AIE) fluorophore and dipicolylamino group as a zinc chelating ligand. To enhance the water solubility of 1 and its selectivity to Zn²⁺ ions, micelles were used to produce a micellar probe. This showed a weak fluorescence at 482 nm derived from TPE. Upon binding with Zn²⁺ in aqueous media at pH 7.4, a large fluorescence enhancement was observed at 530 nm due to an inhibition of photo-induced electron transfer (PET). Further addition of PPI, the fluorescence at 530 nm was gradually decreased while the fluorescence at 474 nm was increased. Thus, we found that the micellar probe 1 showed a high sensitivity and selectivity to Zn²⁺ even in the presence of other competitive biological metal ions along with 45 nM of LOD. Furthermore, the Zn²⁺-chelated probe 1 could be used for the detection of PPI among various anions.



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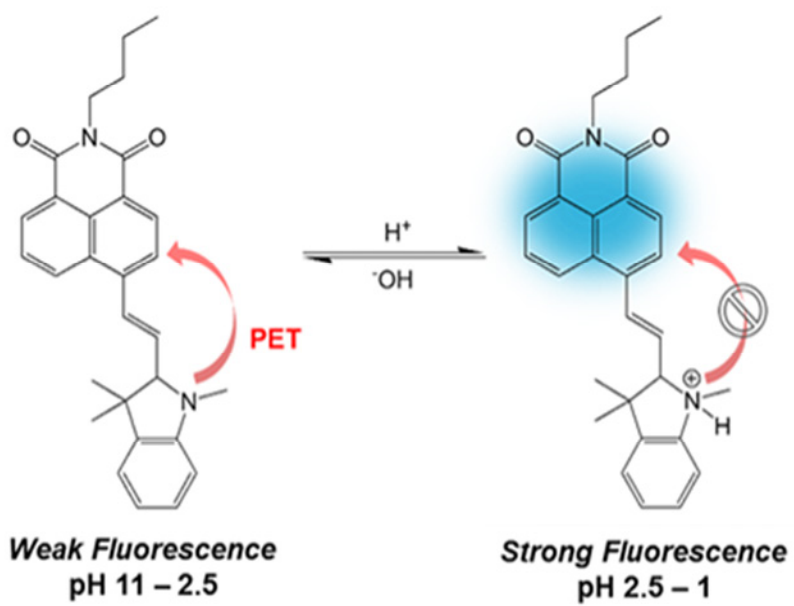
Type: Poster Presentation, Time: FRI 13:00~14:30

A naphthalimide-indoline hybrid: Off-On fluorescent probe for detecting strong acids

Jinju Lee, Min Hee Lee^{*}

Department of Chemistry, Sookmyung Women's University, Korea

We developed a naphthalimide-indoline hybrid (1) as a pH-sensitive turn-on fluorescent probe. Probe 1 displays a weak fluorescence intensity in pH span of 2.5–11.0 owing to a photo-induced electron transfer (PET) from the indoline moiety to the naphthalimide. However, the PET process is suppressed under the pH of 2.5, showing a strong fluorescence signal at 430 nm. The turn-on fluorescent change of 1 is selective for the acidity (H^+) over other anions, metal ions, redox species and it displays a good reversibility. Moreover, glass TLC plates coated with probe 1 can readily detect acid vapors at an ambient atmosphere.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of hemicyanine-based fluorescent probe for the detection of human NAD(P)H:quinone oxidoreductase (hNQO1) activity

Jinju Lee, Min Hee Lee^{*}

Department of Chemistry, Sookmyung Women's University, Korea

We developed a new hemicyanine-based fluorescent probe for detection and imaging of NAD(P)H:quinone oxidoreductase (hNQO1) in human cells. The hNQO1 enzyme is associated with various diseases and it is overexpressed in cancer cells. The probe consist of hemicyanine as a fluorogenic and colorimetric reporter, immolative linker, and trimethyl lock quinone as the hNQO1 enzyme sensitive part. This probe shows a broad absorption band at 480 nm and a very weak fluorescence intensity around 560 nm. However, upon reacting with the hNQO1, a significant increase in the fluorescence intensity and color change from yellow to red were observed in the physiological conditions. In addition, these changes were not observed in the case of other biologically relevant metal ions, redox species, and anions in the similar conditions. Moreover, we found that this probe can selectively detect the hNQO1 enzyme activity with a high specificity constant ($k_{\text{cat}}/K_m = 4.05 \pm 0.753 \times 10^6 \text{ M}^{-1} \text{ min}^{-1}$), which was relatively higher value compared to other probes reported earlier.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Theranostic conjugates for fluorescence and MR imaging and its use for metastatic liver cancer model

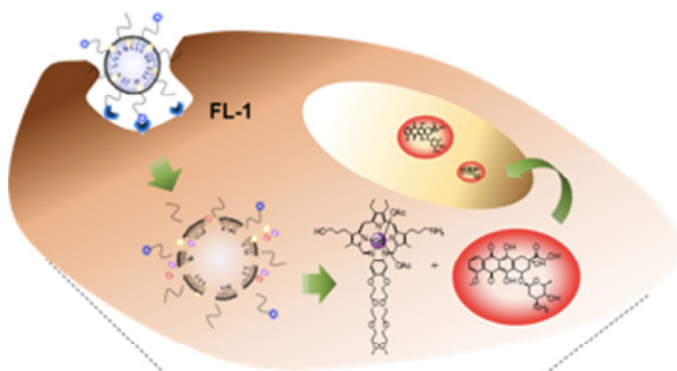
Min Jung Chang, Jongseung Kim¹, Min Hee Lee^{2,*}

Department of chemistry, Sookmyung Women's University, Korea

¹*Department of Chemistry, Korea University, Korea*

²*Department of Chemistry, Sookmyung Women's University, Korea*

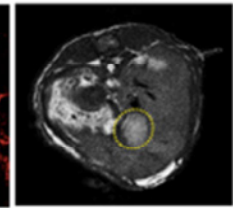
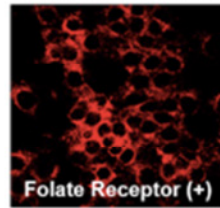
Reported here is a new theranostic agent, **1**, which consists of a Gd³⁺-texaphyrin core conjugated to a doxorubicin prodrug via a disulfide bond. Conjugate **1** was designed to undergo cleavage in the presence of glutathione (GSH), a species typically upregulated in cancer cells. As prepared, conjugate **1** displays no appreciable fluorescence. However, when exposed to excess GSH an increase in the fluorescence intensity at 592 nm is observed that is ascribed to release of free doxorubicin. To improve the solubility and enhance the tumor targeting of **1**, it was loaded into folate-receptor-targeted liposomes to produce FL-1 (for folate liposome loaded with **1**). As inferred from both fluorescence turn on studies and independent HPLC analyses, FL-1 was found to undergo selective uptake and cleavage to release free Dox in the KB and CT26 cell lines, which express folate receptors on the cell surface, relative to the HepG2 and NIH3T3 cell lines, which show low expression of those receptors. FL-1 was found to produce a greater antiproliferative effect in the case of the KB and CT26 cell lines as compared to that in the HepG2 and NIH3T3 cell lines. FL-1 was also found to provide enhanced magnetic resonance imaging in vivo under conditions of T₁ contrast in the early stage of metastatic cancer progression. Finally, time-dependent tumor regrowth studies involving both subcutaneous and metastatic liver cancer mouse models revealed that FL-1 is capable of reducing the tumor burden in vivo.



Imaging

Fluorescence

MRI

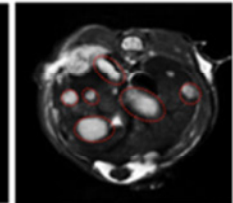
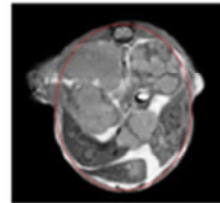


Folate Receptor (+)

Early diagnosis

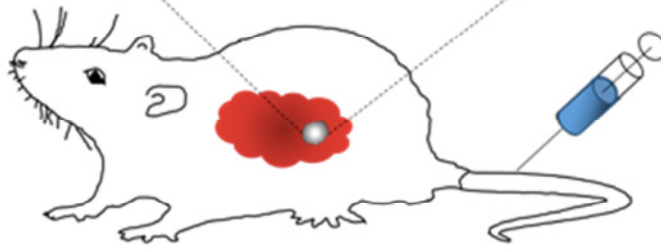
Tumor targeting

Anti-cancer effect



Saline

FL-1



Metastatic liver cancer



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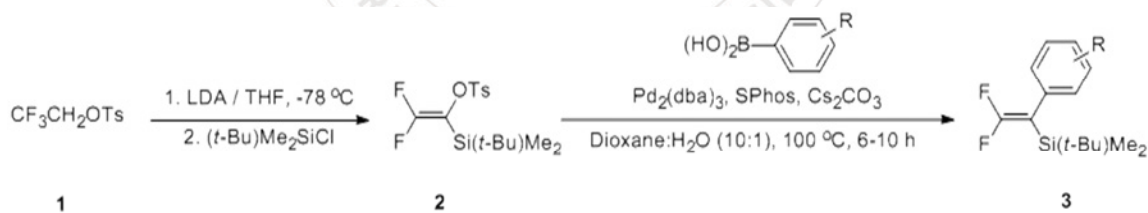
Preparation of 1-(*t*-butyl)dimethylsilyl-2,2-difluorostyrenes

SEOHEE LEE, In Howa Jeong^{1,*}

Chemistry, Yonsei University, Korea

¹*Chemistry and Department of Medical Chemistry, Yonsei University, Korea*

1-(*t*-Butyl)dimethylsilyl-2,2-difluoroethenyl tosylate (**2**) was prepared in 83% yield from the reaction of 2,2,2-trifluoroethyl tosylate (**1**) with 2.2 equiv of LDA in THF at -78 °C, followed by treatment with (*t*-butyl)dimethylsilyl chloride (1.0 equiv). Cross-coupling reaction of **2** with arylboronic acid (2.0 equiv) in the presence of Pd₂(dba)₃ (10 mol%), SPhos (20 mol%) and Cs₂CO₃ (1.7 equiv) in a cosolvent of dioxane and H₂O (10:1) at 100 °C for 6-10 hours afforded the coupled product **3** in moderate to good yields. The scopes and limitations of this reaction will be presented.



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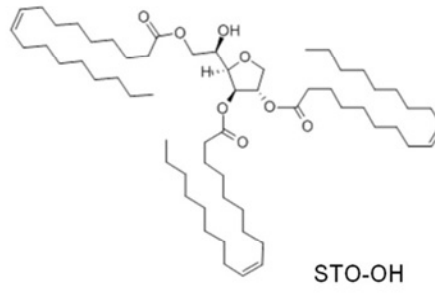
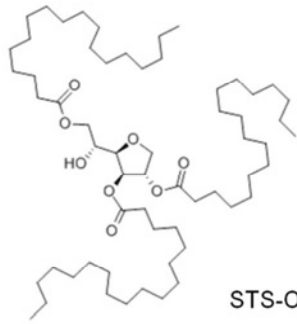
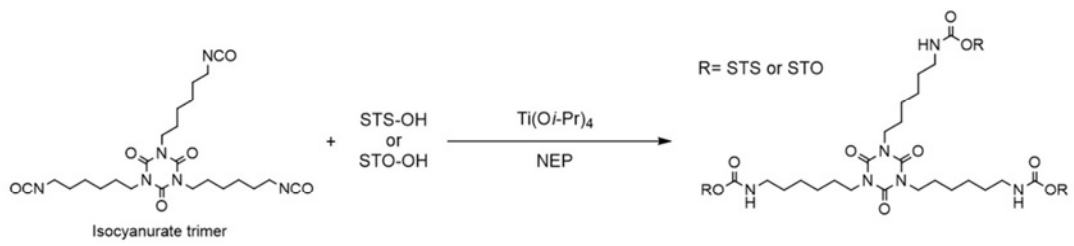
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and application of 3D-water repellent materials for development of highly durable non-F-containing water repellent agents for textiles

Kun Hee Kim, Jaewoong Kim, Seung Eun Lee, Jin Wook Han^{*}, Chang Ho Oh^{*}

Department of Chemistry, Hanyang University, Korea

Water repellent agents for textiles include F-containing water repellent and non-F-containing water repellent. Due to a small atomic radius and high electronegativity of fluorine atom, F-containing water repellent agents have suitable properties for water repellent materials, such as non-adhesiveness, water repellency, oil repellency, and heat resistance. However, F-containing water repellent agents have a great disadvantage of environmental concern from PFC (perfluorinated compound). Herein, we wish to report eco-friendly urethane-based non-F-containing water repellent agents in order to replace F-containing water repellent agents. The characteristic of the urethane-based non-F-containing water repellent agents is that it does not contain PFC and is excellent in repellency against contaminants as well as water. It exhibits excellent water repellency as compared with conventional wax, silicone and polyacrylic water repellent agents. In addition, it has a good process stability and excellent washing durability in natural drying conditions. Non-F-containing water repellent agents were prepared from isocyanurate trimer (1.0 equiv) and STS-OH or STO-OH (3.0 equiv) in the presence of Ti catalyst (1 mol %) in NEP (N-ethylpyrrolidone) for 15 h at 50 °C.



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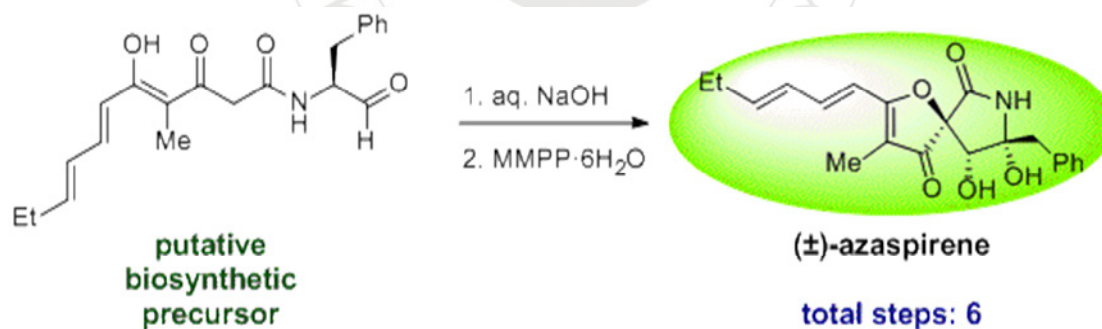
Type: Poster Presentation, Time: FRI 13:00~14:30

Six-Step Total Synthesis of Azaspirene

Deokhee Jo, Sunkyu Han^{*}

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

The total synthesis of (±)-azaspirene was achieved in a total of six steps from commercially available materials. Keys to the conciseness of our synthetic approach were the effective γ -lactam formation from linear precursor and successful tandem epoxidations of γ -lactam to afford α,β -epoxy- γ -hydroxy- γ -lactam intermediate. While our streamlined synthesis of azaspirene sought inspiration from its biogenetic hypothesis, experimentally observed chemical reactivity of biosynthetically relevant precursors conversely provides insights to the biological origin of this natural product.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Coordination-driven self-assembly of trigonal cages using new triazole-based tripodal ligand

JATINDER SINGH, DONGHWAN KIM, Kiwhan Chi*

Department of Chemistry, University of Ulsan, Korea

Coordination-driven self-assembly process, which is able to construct 3D supramolecular architectures, exhibits great potential in catalysis, drug-delivery and encapsulation. Triazole, a five membered heterocycle has important role in several biological and chemical processes. Triazole-based ligands are useful building blocks and linking units in coordination chemistry. The present work demonstrates the synthesis, characterization and encapsulation studies of trigonal cages based on triazole-based donor and arene-Ru(II) acceptors. All the new complexes have been characterized by various spectroscopic techniques.

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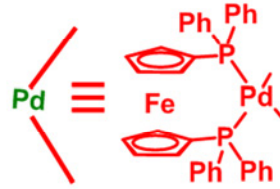
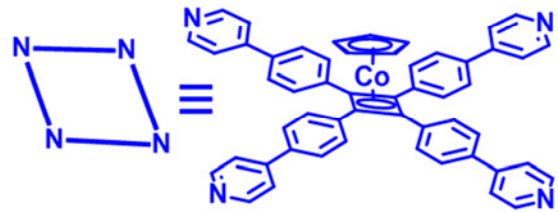
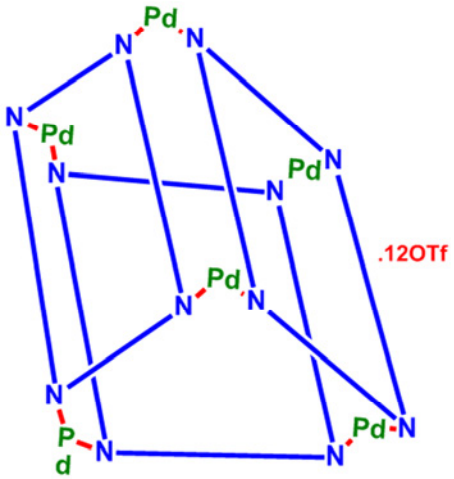
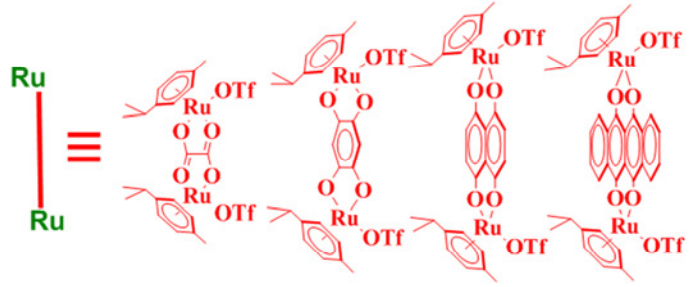
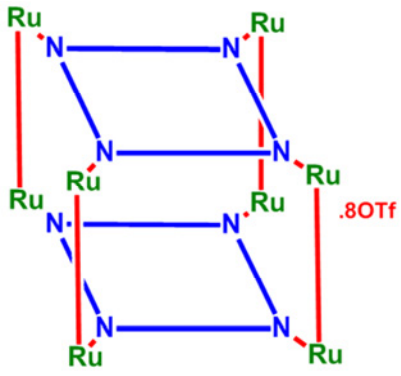
Type: Poster Presentation, Time: FRI 13:00~14:30

Coordination-driven self-assembly of cubes and trigonal prism using new cobalt sandwich based tetrapodal ligand: Synthesis, characterization and encapsulation studies

JATINDER SINGH, DONGHWAN KIM, Kiwhan Chi*

Department of Chemistry, University of Ulsan, Korea

Coordination-driven self-assembly process used for the synthesis of 2D and 3D molecular architectures has been of great importance owing to their application in catalysis, drug-delivery and encapsulation. Cobalt sandwich based tetrapodal ligand has unique properties to construct face-based conformational isomers by directing the cyclopentadiene unit inside or outside of the cage. Herein, we describe the synthesis of supramolecular cages, which possess cubic and trigonal prism geometry and subsequently use them for the encapsulation of various guest molecules.



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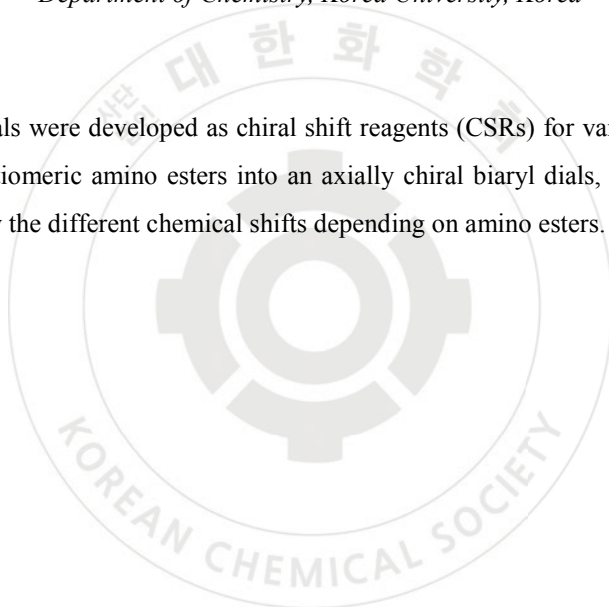
Type: Poster Presentation, Time: FRI 13:00~14:30

chiral shift reagents (CSRs)

Ghi-Sung Lee, Seong-eon Lee, soobin Kim, eunjeong jeong, Hogyu Han*

Department of Chemistry, Korea University, Korea

Axially chiral biaryl dials were developed as chiral shift reagents (CSRs) for various amino esters. Upon introduction of the enantiomeric amino esters into an axially chiral biaryl dials, the diastereomeric imines were obtained and show the different chemical shifts depending on amino esters.



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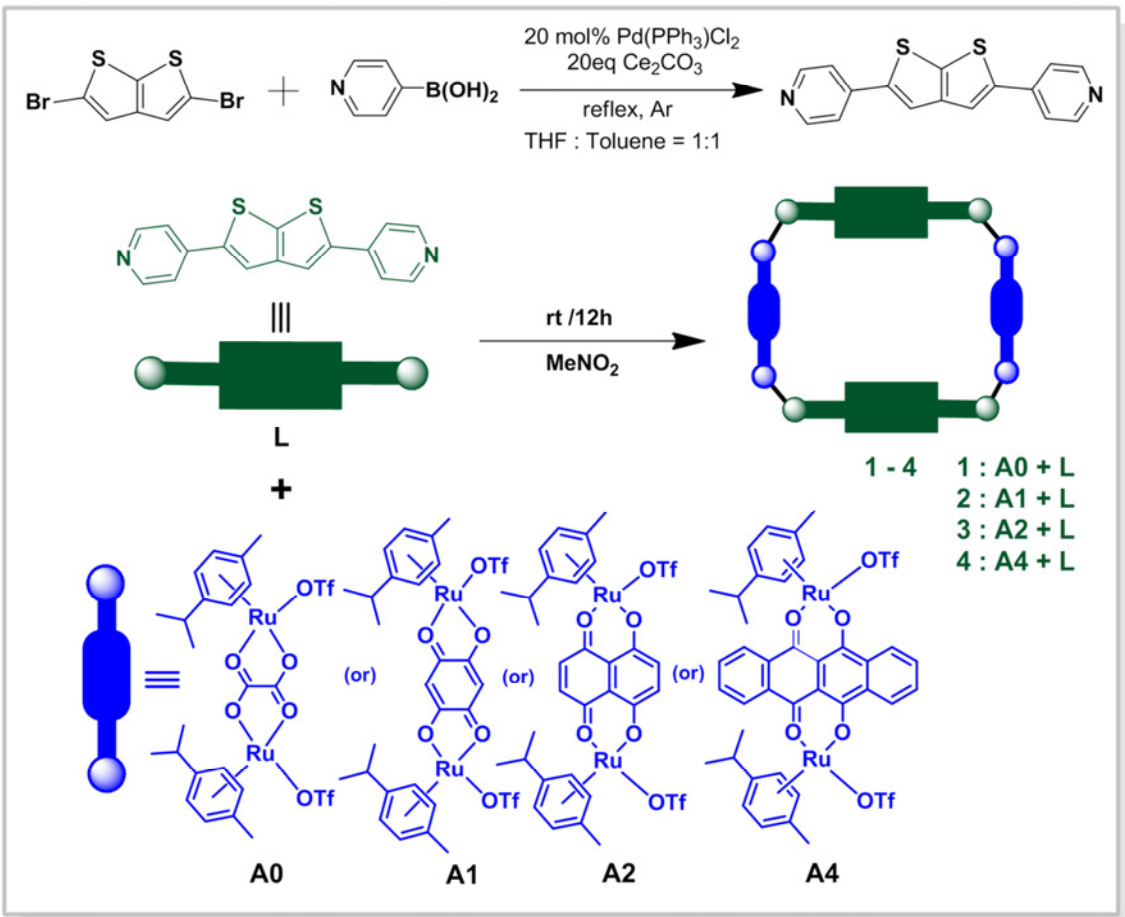
Type: Poster Presentation, Time: FRI 13:00~14:30

Self-assembly of thieno[2,3-*b*]thiophene-derived pyridyl ligand and arene-Ru(II) based acceptors

DONGHWAN KIM, Kiwhan Chi*

Department of Chemistry, University of Ulsan, Korea

In recent years, coordination-driven self-assembly has been utilized in the synthesis of complex molecular topologies such as Solomon links, Hopf's links and Borromean rings. Our group has also reported a number of self-assembled interlocked architectures using highly conjugated thiophene based electron rich donors and tetracene-based Ru(II) acceptor. Thiophene possesses the highest resonance energy among the five membered heterocycles. In addition, two or three annulated thiophene rings are also known for various applications such as functional materials and photosensitization. Herein, we report the synthesis of a new ligand and four metallamacrocycles self-assembled with thieno[2,3-*b*]thiophene donor and arene-Ru(II) acceptors. All the new compounds are fully characterized with various spectroscopic techniques.



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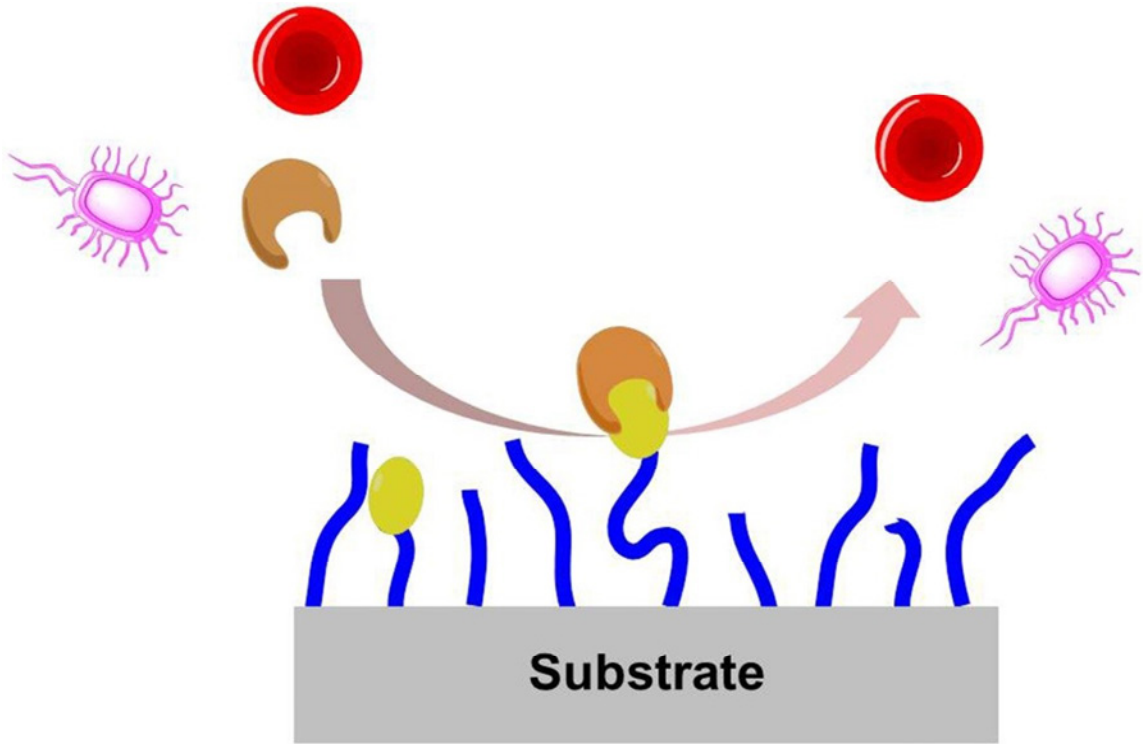
Surface Organic Chemistry for Chemically Functionalizable, Non-Biofouling Surfaces

Young Hwan Jung, Gyeongyeop Han¹, JungKyu Lee^{1,*}

Department of Bio Nano Materials, Bio Campus of Korea Polytechnics, Korea

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

Biofouling, the deterioration of device and surface function resulting from the accumulation of biological matter (i.e., proteins, cells, and microorganisms), is an important issue in a wide range of fields, including biosensors, biomedical devices, medical implants, marine equipment, water purification, and drug delivery carriers.¹ Given the fact that the biofouling is a universal and problematic phenomenon, such as low signal-to-noise ratios for immunoassays and harmful side effect for biological implants, it is necessary to introduce functionalities on solid surfaces (e.g., silicone, gold, and polymer surfaces), which minimize the unwanted, non-specific adsorption of bioentities as well as improve the device function.² Therefore, many studies have been reported how to reduce the nonspecific adsorption of bioentities on the surfaces. Recently, it has been found that non-biofouling coating on biocompatible polymers, such as poly(ethylene glycol) (PEG) derivatives and zwitterionic polymers, is one of the best methods to minimize the biofouling on solid surfaces as shown in Figure 1.^{3,4} Herein, we present non-biofouling polymer coatings polymerization on gold, silicone and cyclic olefin copolymer surfaces, using surface organic reactions and surface-initiated, atom transfer radical polymerization. The formed polymeric coated substrates are characterized by water contact angle, ellipsometric thickness, and X-ray photoelectron spectroscopy (XPS). Moreover, the non-biofouling performance of the substrates is investigated by scanning electron microscopy (SEM) and fluorescent microscopy. We believe that the strategy used herein will not only widen the application of non-biofouling coating on solid surfaces to biosensors and medical devices, but also be applicable to various other substrates which need to be functionalized spatioselectively for their applications.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Metal-Free Esterification of Aldehyde Using Bromo Source under Mild Condition

Hee-Kwon Kim

Department of Nuclear Medicine, Chonbuk National University Medical School and Hospital, Korea

Ester is common chemical functional group found in various natural products, pharmaceuticals, and polymers. The ester unit has been utilized to a variety of organic synthesis fields. Nucleophilic substitution reaction of carboxylic acids with alcohols is widely used methods for the synthesis of esters. In addition, oxidation of aldehydes to esters using hemiacetal intermediate is one of the useful methods. However, the synthetic methods have a weakness such as steric effect and instability of intermediate. Herein, novel method for the conversion of aldehydes to esters is described. In the novel synthetic method, acyl bromide intermediates was prepared by the treatment of aldehydes with bromo source, and then were reacted with various alcohols and phenols to give the corresponding esters with high yields under mild reaction condition.

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Area: Organic Chemistry

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Highly Selective Recognition of Oxoanions by a Molecular Cage

Juhyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new molecular cage was synthesized containing both hydrogen bonding donors such as amides and pyrroles and hydrogen bonding acceptors of imines. It was proved by ¹H NMR and UV/Vis spectroscopic analyses that this three dimensional receptor is able to bind oxoanions such as dihydrogen phosphate, pyrophosphate, hydrogen sulfate, and sulfate (as their tetrabutylammonium salts) with high selectivity and affinity relative to other anions including halide anions. The single crystal X-ray diffraction analysis showed that the receptor forms a 1;1 complex with the dihydrogen phosphate where the two hydrogen atoms of the anion forms hydrogen bonds with the nitrogen atoms of imine of the cage with the amide and pyrrolic NH being hydrogen-bonded to the oxygen atoms of the anion.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-277**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Diazo-coupled calix[4]arene-Strapped Calix[4]pyrrole: a Colorimetric Sensor for Specific Ion Pairs

Kim Seung Hyeon, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A chromogenic ion pair receptor was synthesized on the basis of a diazocalix[4]arene and calix[4]pyrrole hybrid compound. In this case, the calix[4]arene subunit was locked in the con conformation whereas the calix[4]pyrrole constituent are conformationally flexible. It was found by UV/vis and ¹H NMR spectroscopic analyses that the ion pair receptor is highly selective for calcium and fluoride ion. For example, upon the addition of these ions to the solution of the receptor, drastic color change was observed presumably as the result of formation of the ion complexes by the receptor. In these ion complexes, the fluoride anions were bound to the calix[4]pyrrole via hydrogen bonding interactions with the pyrrolic NHs whereas the calcium cation was complexed with the oxygen and nitrogen atoms of the calix[4]arene and the triazole group, respectively. Especially, the color change of the receptor solution from red to orange is ascribable to the calcium ion bound to the oxygen atoms of the phenolic groups of the calix[4]arene linked to the diazo groups. By contrast, the color change by the fluoride anion form yellow to blue is presumably attributed to deprotonation of the phenolic OH the calix[4]arene by the basic fluoride anion.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-278**

Area: Organic Chemistry

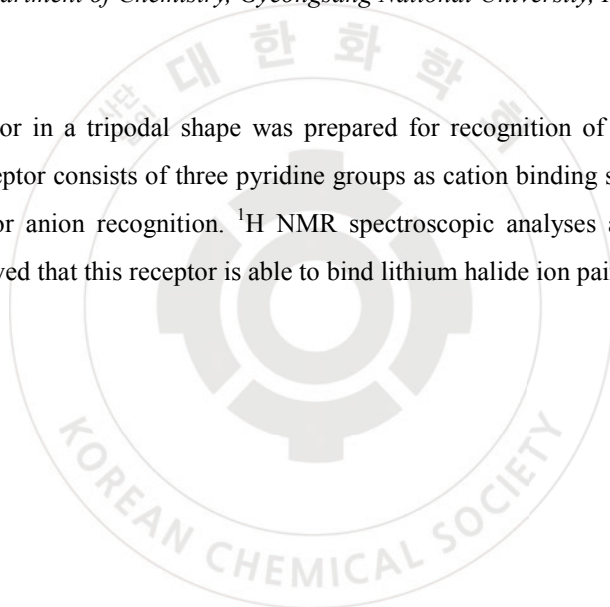
Type: Poster Presentation, Time: FRI 13:00~14:30

A tripodal ion pair receptor for selective recognition of lithium salts

juho yang, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

.A new ion pair receptor in a tripodal shape was prepared for recognition of ion pairs containing the lithium cation. The receptor consists of three pyridine groups as cation binding sites linked via amides to three pyrrole groups for anion recognition. ¹H NMR spectroscopic analyses and single crystal X-ray diffraction analysis proved that this receptor is able to bind lithium halide ion pairs highly selectively over other alkali metal salts.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-279**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A calix[4]pyrrole crown ether having a deep cavity and its ion pair recognition

Hye Jin Han, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new ion pair receptor based on calix[4]pyrrole strapped with a crown ether was prepared. This receptor consists of calix[4]pyrrole having four phenoxy walls in its meso carbons and a crown ether linking two diagonal or neighboring phenol groups. This ion pair receptor was found to be able to bind alkali metal fluoride salts selectively over other anion salts. ¹H NMR spectroscopic analysis provided evidence that alkali metals are bound to the crown ether ring with the fluoride anion being hydrogen-bonded to the pyrrolic NHs. ¹H NMR titration of the receptor with alkali metal fluoride salts proved that this ion pair receptor binds these salts with high affinity in a 1:1 stoichiometry.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-280**

Area: Organic Chemistry

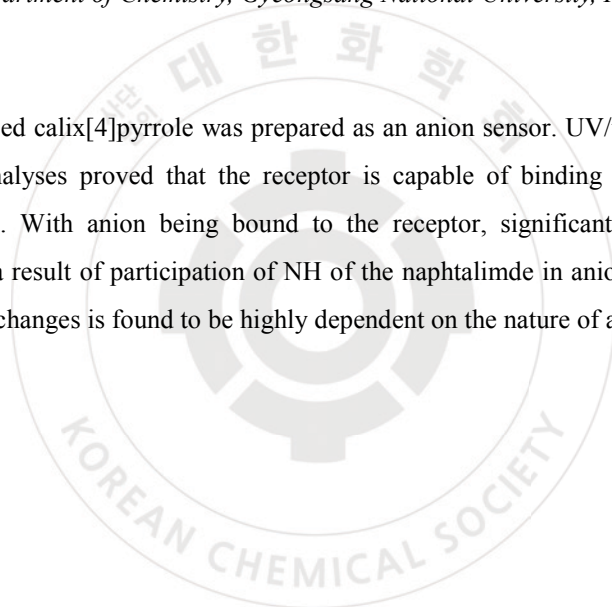
Type: Poster Presentation, Time: FRI 13:00~14:30

A new fluoro- and chromo-genic anion sensor based on calix[4]pyrrole

JeongHyeon Kim, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A naphthalimide-strapped calix[4]pyrrole was prepared as an anion sensor. UV/vis, fluorescence, and ^1H NMR spectroscopic analyses proved that the receptor is capable of binding halide anions with high affinity and sensitivity. With anion being bound to the receptor, significant color and fluorescence changes took place as a result of participation of NH of the naphthalimide in anion binding. The extent of color and fluorescence changes is found to be highly dependent on the nature of anions in question.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-281**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Heteromultitopic Ion Pair Receptor Based on 1,3-Alternate Calix[4]-Crown-5 Appending Dipyrrolylquinoxaline

Han-byeol Choi, Sung Kuk Kim *

Department of Chemistry, Gyeongsang National University, Korea

A new heteromultitopic ion pair receptor consisting of 1,3-alternate calix[4]arene crown-5 connected with two dipyrrolylquinoxaline(DPQ) via the amide linkers was synthesized. It was proved by ¹H NMR spectroscopic analyses and UV-vis spectra that this receptor is able to bind the potassium cation as well as several anions such as the fluoride and the dihydrogen phosphate anion. In this case, the potassium cation is bound to the calix[4]arene crown-5. By contrast, the anions are hydrogen bonded to the pyrrolic NH of DPQ resulting in color changes. Binding property of the receptor for specific anions and cations as well as ion pair will be presented in detail.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-282**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile Synthesis of Diphenylmethyl esters using 2-Diphenylmethoxy-1-methylpyridinium Triflate under mild condition

Minh Thanh La, Hee-Kwon Kim^{1,*}

Department of Medical Science, Medical School, Chonbuk National University, Korea

¹*Department of Nuclear Medicine, Medical School, Chonbuk National University, Korea*

Protection and deprotection of esters are one of the most important methodologies in organic synthesis. Diphenylmethyl group has been widely used as a protecting group for carboxylic acids. Here, Novel practical method for the conversion of carboxylic acids to diphenylmethyl (DPM) esters is described. DMP esters were synthesized through the reaction with 2-diphenylmethoxy-1-methylpyridinium triflate intermediates which were formed in situ from the treatment of MeOTf and 2- diphenylmethoxy-1-methylpyridinium. Using this reaction protocol, various diphenylmethyl (DPM) esters were prepared with high yields under mild condition. This effective method is highly effective method for the synthesis of DMP esters, and offers a promising approach for facile esterification of a variety of carboxylic acids.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-283**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Colorimetric Transition of Systemized Functional Group Controls in Polydiacetylenes

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¹*School of Integrated Oriental Medical Bioscience, Semyung University, Korea*

Polydiacetylenes (PDAs) are unique micelle type polymeric, molecular system, which are containing diacetylene functional group in molecules. These specific vesicles could be polymerized from diacetylene containing linear molecules with UV irradiation and ultrasonic treatments in aqueous media. And this photopolymerization of diacetylene forms an array of acetylene-ethylene backbone with delocalized π -electrons. The polymerized vesicle solution with these compounds showed blue to purple or red or yellow colorimetric transitions by external stimuli such as temperature, pH, molecular or ion contact, solvent, and etc. Since the color changes of PDAs are detectable by naked eyes, it has been developed label free sensor for variable stimuli.¹

Recently we have designed and synthesized PCDA (pentacosanoic acid) derivatives, which have different side alkyl chain lengths of head group. These series of PCDA derivatives showed different colors (blue, purple, red and yellow) at room temperature without external stimuli. In addition, we have performed that the functionalization of PCDA molecules with a series of polar or non-polar functional groups. The polarity-controlled PCDA molecules show an elevation of color-changing (blue to purple and red) temperature. We believe that these two experimental findings allow many insights to understand color changing mechanism of PDAs.²

Reference 1. X. Chen, J. Yoon, *Dyes Pigments*, **2011**, *89*, 194.

2. N. Han, H. J. Woo, S. E. Kim, S. Jung, M. J. Shin, M. Kim, J. S. Shin, *J. Appl. Poly. Sci.* **2017**, *134*, 45011.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-284**

Area: Organic Chemistry

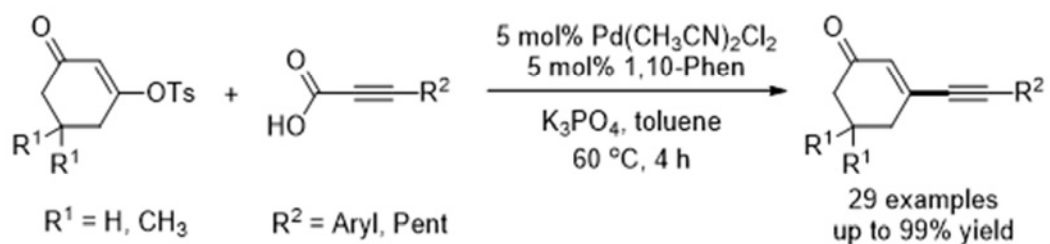
Type: Poster Presentation, Time: FRI 13:00~14:30

Pd-catalyzed decarboxylative coupling reaction of alkynyl carboxylic acid and alkenyl tosylate

subeen yu, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Conjugated enynes have been not only found in the electro- and optical materials natural compounds, and pharmaceuticals but also employed as useful synthetic building blocks due to the fact that they can be diversely transformed into the important moieties. Among them, conjugated enynones have been attracted attention in the synthesis of bioactive agents and used as starting materials for the preparation of useful organic molecules such as allene, cyclooctatetraene, pyrrolizine, chromene, fused ring and polycyclic compounds. Among synthetic methods for enyne, Sonogashira type coupling reactions of 3-oxoalkenyl halides (or pseudo halide) and terminal alkyne has been widely used as a straightforward tool. However, the reaction with 3-oxoalkenyl tosylate was very rare even though alkenyl tosylate was easily accessible and stable. Moreover, the coupling reaction with alkynyl carboxylic acid has never been reported so far. Herein we report the decarboxylative coupling reaction of alkynyl carboxylic acid and 3-oxoalkenyl tosylates. A variety of alkynyl carboxylic acids were coupled with 3-oxocyclohexenyl tosylates to provide the corresponding enynones in good to excellent yields. Alkenyl tosylate is readily prepared, stable and cost efficient. This catalytic system is phosphine free and showed good tolerance toward functional groups such as chloride, cyano, nitro, ester, aldehyde and alcohol. In addition, it was found that phenylpropionic acid showed higher reactivity in the reaction with alkenyl tosylate than phenyl acetylene.



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Code: **ORGN.P-285**

Area: Organic Chemistry

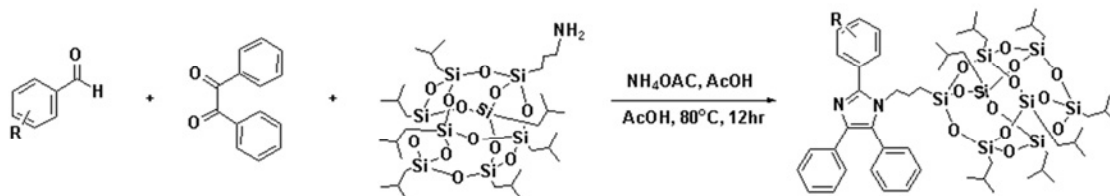
Type: Poster Presentation, Time: FRI 13:00~14:30

synthesis of various functionalized imidazole derivatives incorporated to POSS

kyung-min choi, Dong-Soo Shin *

Department of Chemistry, Changwon National University, Korea

The synthesis of N-substituted POSS-imidazoles in one pot typically prepared using the condensation method from diketones and aminopropylisobutyl-POSS. A wide variety of functional groups and substitution patterns were tolerated under the present procedure, and moderate yields were obtained for aminopropylisobutyl-POSS. We also found that the resulting compounds were valuable product allowing for the elaboration to OLED, DSSC building blocks.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-286**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Facile Synthetic Method for the Preparation of Indene Derivatives with Thioester

Hee-Kwon Kim

Department of Nuclear Medicine, Chonbuk National University Medical School, Korea

Indene unit is a commonly found in a variety of pharmaceuticals and natural compounds. Many structures of indene based derivatives have biological activities and have been used for drug discovery. However, indene derivatives were prepared via long synthetic steps. Herein, an efficient preparation of indene derivatives containing thioesters is described. Synthesis of indene containing thioesters was easily performed by the treatment of diazo-compounds with aldehydes and thiols. In the present study, a variety of indene derivatives were produced via one-pot reaction protocol in high yields. Our protocol will be a promising approach for the synthesis of various indenenes for biological active compounds.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-287**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Self-Assembled Organic Microfibers and Nanorods of 2,6-Diphenyl substituted dipyrrolopyrazine (DPP) derivatives for Optoelectronic Applications

Puttavva Meti, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Microfibers with promising application in optoelectronics are desirable in current material synthesis. Synthetic method has been developed for the preparation of dipyrrolopyrazine derivatives by employing palladium catalysed Buchwald and Sonogashira coupling reactions. A comprehensive study on the synthesis, optical properties, thermal stability and morphology of 1,5-dimethyl-2,6-diphenyl-1,5-dihydropyrrolo[3,2-*b*:3',2'*e*]pyrazine derivatives (DPP) were carried out. SEM analysis shows the formation of microfibers, square facets and nanorods. Electrochemical studies revealed HOMO energy levels in the range of -5.68 to -5.95 eV and LUMO energy levels in the range -2.90 to -3.34 eV, respectively. All the compounds exhibited a high degree of thermal stability and decomposition temperature of 322–372 °C. The enhanced air and thermal stability combined with good morphological properties make DPP a promising candidate for future optoelectronic applications.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-288**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of novel Amino pyranoses and Amino nortropinones

Eon Jin Lee, songmi Bae, Dai Il Jung*, JUNGTAI HAHN¹

Department of Chemistry, Dong-A University, Korea

¹*Department of Beauty Care, U1 Univerysity, Korea*

Tropane alkaloids have received a lot of attention because of their remarkable pharmaceutical significance. Tropane alkaloids are a kind of bicyclic [3.2.1] alkaloids. 8-Azabicyclo[3.2.1]octan-3-ones can act as anticholinergics or stimulants. Pyranose derivatives possess antiviral activity with low side effects. pyranose derivatives aid security and defense operations by forming molecular codes on the surfaces of cells that identify whether the cell is one of our own or an intruder. Our group has been interested in exploiting the unique properties of pyranose scaffolds to develop bioactive peptide analogs to discover systematic bioactive drugs while decreasing unwanted side effects. In our lab, 8-azabicyclo[3.2.1]octan-3-ones can be obtained by the reaction of diamines(2,3-diaminopyridine or 3,4-diaminotoluene, etc), 2,5-dimethoxy-tetrahydrofuran, and 1,3-acetonedicarboxylic acid. And pyranose derivatives can be obtained by the treatment of diamines(1,6-diaminohexane or 1,12-diaminododecane, etc) and pyranoses (mannose) in anhydrous methanol.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-289**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of 1H-benzo [b] [1,4] benzodiazepine derivatives by Using silica sulfuric acid

do hun Lee, Ji Song Park, Dai Il Jung*, JUNGTAI HAHN¹

Department of Chemistry, Dong-A University, Korea

¹*Department of Beauty Care, UI-University, Korea*

Benzodiazepines are interesting compounds that can enhance the efficacy of neurotransmitter GABA, and therefore benzodiazepine derivatives are used as sedatives or anticonvulsants. Benzodiazepines with anticonvulsant activity include Clonazepam, Diazepam, and Lorazepam. Benzodiazepines with active antioxidants include Bromazepam, Etizolam, and oxazepam. Despite the various pharmaceutical, industrial and synthetic applications, the synthesis of 1H-benzo [b] [1,4] benzodiazepines received relatively less attention than 1H-benzo [e] [1,4] benzodiazepines. The core of this study is to synthesize 1H-benzo [b] [1,4] benzodiazepine derivatives by reacting various ketones, heteroaromatic ketones, and oximes with diamines. The direct reaction of diamines and oximes did not occur. We have found that Dichloramine-T and Amberlyst-15 can be converted to oximes to the corresponding carbonyl compounds. And we tried to synthesize 1H-benzo [b] [1,4] benzodiazepine derivatives by using silica sulfuric acid as an efficient and reusable reagent.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-290**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Efficient preparation method of 2,6-disubstituted-4-hydroxy benzoate

Dahye Kim, Sangho KOO^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

In an effort to synthesize carotenoids with improved biological activity, we developed a practical synthetic method of diversely R-substituted 4-hydroxybenzoic esters as the terminal ring structure. A practical two-step synthetic method of diversely R-substituted 4-hydroxybenzoic esters, which may have wide applications in household chemicals and polymeric materials, was developed by 2:1 coupling between ethyl acetoacetate and aldehydes (RCHO) in t-BuOK/t-BuOH, followed by oxidative aromatization of the resulting Hagemman's esters by using stoichiometric NBS and catalytic TMS.OTf.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-291**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Durable benzenesulfonyl protection for phenols- efficient synthesis of polyphenols

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¹*Department of Chemistry, Myungji University, Korea*

A robust repertoire for phenol protection/deprotection was demonstrated by the use of durable benzenesulfonyl group, which survives many harsh reaction conditions using Grignard reagents, organolithium reagents, metal alkoxides, phosgenes, mineral and Lewis acids etc. A facile deprotection condition utilizing pulverized KOH and t-BuOH in hot toluene make this protocol as a practical method which can be applied to the multi-step synthesis of biologically and medicinally important poly phenol compounds.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-292**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of 9,9',13,13'-tetra-Phenyl-substituted-carotenoids

Hyebin Yoo, Sangho KOO^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Unnatural carotenoids containing various Phenyl substituents provide advantages in terms of stability and electronic characteristics, compared with the natural carotenoids. Carotene with tetra-Phenyl substituents has better electrical conductivity than carotene with di-Phenyl substituents. Carotenoid molecular wires containing tetra-Phenyl substituents can be assembled by the Wittig reaction between tetra-Phenyl-substituted-dial and 4-thiomethylbenzyl phosphonium bromide(Wittig salt). tetra-Phenyl-substitued-dial can be effectively synthesized by the Julia-Kocienski olefination of the Phenyl-substituted-C5 - BT(benzothiazole)-sulfone with C10 2,7-diphenyl-2,4,6-octatrienedial.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-293**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A study on the synthetic method for organic molecular nanowire

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Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Nowadays organic molecular nanowires for the smaller, faster, and flexible substitutes for the conventional metallic wire. Organic molecular wires with variable conductance is one of the urgent goals in molecular electronics. Organic molecules containing terminal thiol group can be used in electronic conductance using Atomic Force Microscopy(c-AFM). Carotenoids structure is an ideal organic molecular wire of potentially high electric conductance. Existence of extensive π -conjugation offer high electronic conductance because of the delocalized π -electron system. We synthesized the carotenoid molecular wires containing terminal thiol group by sulfone-mediated coupling, Ramberg-backlund and double elimination reaction between allylic sulfone and C10-dichloride. We were able to synthesize various molecular wires based on the carotenoid structure and compare the electronic conductance of various molecular wires.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-294**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Study on the Mn(III)-initiated radical oxidation and the application on the synthesis of natural products

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¹*Department of Chemistry, Myungji University, Korea*

Abstract: A new type of terpenoid cyclization directed by a β -keto ester moiety has been developed, which proceeded by manganese(III)-initiated oxidation of the β -keto ester, followed by an intramolecular hetero Diels-Alder reaction with the terpenoid chain. Based on the mechanism of two steps oxidation, we improved the reaction to be catalytic by the addition of a second cobalt(II) oxidant. A high yield was gained under the condition of 5 mol% $\text{Mn}(\text{AcO})_3$ and 2 mol% CoCl_2 . For application, 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.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-295**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A study of synthetic method for Unnatural carotene wire

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Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Unnatural carotenoids containing various phenyl substituents compared with Natural carotenoids in terms of stability as well as electronic characteristics. We have perfectly demonstrated the efficient synthesis of natural carotenoids, which can be further extended to the synthesis of unnatural carotenoid wires. The unnatural carotenoids can be assembled by the coupling and double elimination reaction between haloallylic sulfone with dialdehyde unit. allylic sulfone moiety attaching aromatic phenyl groups containing para-substituents X(OMe, Me, H and Cl) can be prepared from acetophenone derivatives. Therefore, We were able to measure electrical conductivity for various carotenoid wires.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-296**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

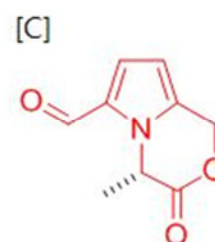
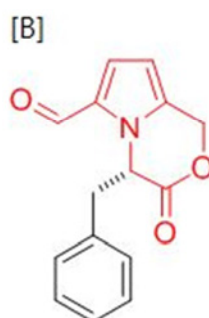
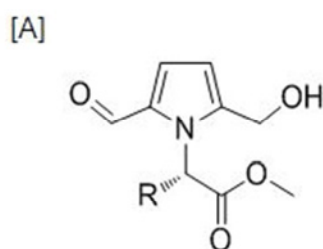
Synthesis of Various substituted Pyrrole compound

Ik Joon IN, Sangho KOO^{1,*}

Department of Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

A effective conversion method of carbohydrates into N-substituted 5-hydroxymethylpyrrole-2-carbaldehydes (pyrralines) was developed by the reaction with primary amines and oxalic acid in DMSO at 60~90 oC. Further cyclization of the highly functionalized pyrralines afforded the pyrrole-fused poly heterocyclic compounds as potential intermediates for drugs, food flavors, and functional materials. The mild Maillard variant of carbohydrates and amino esters in heated DMSO with oxalic acid expeditiously produced the pyrrole-2-carbaldehyde skeleton[A], which can be concisely transformed into the pyrrole alkaloid natural products[B], [C].[B] and [C] have been used for pain-reliever in traditioanl folk medicine. Further reach is focused on sythesizing various substituted pyrrolo-lactone compounds as potential drug candidates



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-297**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Oxidative deacetylation of β -keto esters and its application to heterocyclic compound synthesis

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¹*Department of Chemistry, Myungji University, Korea*

Oxidative deacetylation of β -keto esters, using Mn(III)/Co(II) catalysts under aerobic condition, can generate α -oxo esters. The subsequent intramolecular Diels-Alder reaction or Paal-Knorr type cyclization, depending on the δ -carbon substitutional pattern, may produce dihydropyran or furan derivatives, respectively. Modification of the reagent combination and diversification of the β -keto ester starting materials will expand the application of this method to the synthesis of various furan, pyrrole, thiophene and indole containing natural compounds.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-298**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of Oseltamivir Derivatives as Inhibitors of Influenza Neuraminidase

Hee-Kwon Kim

Department of Nuclear Medicine, Medical School, Chonbuk National University, Korea

Influenza A virus is known as the family of Orthomyxoviridae. Millions of people are infected by Influenza virus, and their lives are threatened. Therefore, humans have an increasing concern about the infection from influenza virus, and made extensive efforts to discover effective treatments. Oseltamivir is the first orally available drug which was marketed in 2000. In this study, neuraminidase inhibition constants were calculated for several novel oseltamivir derivatives to get better active drug structure against influenza virus than oseltamivir. According to the value of neuraminidase inhibition constants, novel oseltamivir derivatives were chosen and synthesized from commercially available cheap materials. These synthetic procedures were practical, and allowed to develop potential anti-influenza drugs with good overall yield.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-299**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Isoquinoline derivatives by microwave-assisted Pd-, Cu-catalyzed coupling reaction

A Reum Park, Eul Kgun Yum *

Department of Chemistry, Chungnam National University, Korea

Isoquinoline derivatives have become interesting substances as a starting material for drugs owing to biological activities, but diversification of isoquinoline is very limited in the literatures. We need to construct diversification of isoquinoline derivatives with rapid and efficient synthetic methods for various structural modification for biological tests. In this work, we studied the synthesis of isoquinoline derivatives under microwave-assisted palladium-, copper-catalyzed synthetic techniques with Suzuki, Heck, Sonogashira and Ullmann-type *N*-arylation reaction. Microwave irradiation provides advantage of reducing reaction time and promoting yield.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-300**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Characterization of New Hole-Blocking Materials Using Pyrimidine and Phenylene Segments for Blue Phosphorescent Organic Light-Emitting Diodes

SEOKHOON JANG, YOUNGU LEE*

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

Recently, phosphorescent organic light-emitting diodes (OLEDs) have received a great attention because they can harvest singlet and triplet exciton. In the case of blue phosphorescent OLEDs, their efficiency is still lower than red and green OLEDs. One of the biggest problems of their low efficiency is the leakage of hole and triplet exciton in the emitting layer (EML). If the highest occupied molecular orbital (HOMO) energy level of the electron-transporting layer (ETL) adjacent to the EML is higher than that of emitting materials, the hole can be migrated into ETL. In addition, if the triplet energy is lower than that of emitting materials, the ETL can quench the triplet energy. In order to confine the hole and triplet exciton in the EML, hole-blocking materials (HBMs) having a high triplet energy and deep HOMO energy level must be introduced between the EML and ETL. Furthermore, it is well known that low glass transition temperature (T_g) characteristics of OLED materials tend to shorten the device lifetime due to thin film crystallization during OLED driving. Therefore, new HBMs with high T_g as well as high triplet energy and deep HOMO energy level must be developed. In this work, we designed and synthesized two HBMs using pyrimidine and phenylene segments. The thermal and optical, electrochemical, and electron-transporting characteristics of two materials were investigated by using thermogravimetric analysis, differential scanning calorimetry, UV-Vis spectroscopy, and cyclic voltammetry and by fabricating electron-only device. The device performance based on new HBMs will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-301**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

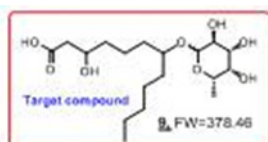
Total synthesis of a natural product for the treatment of diabetic complications

Jung Youl Park*, Eunju Jeong¹, Jeong In Yun¹

Dept. of Applied Chemistry, Daejeon University, Korea

¹*GH BIOTECH, Korea*

Diabetes is a metabolic disorder of multiple etiologies that characterizes chronic hyperglycemia resulting from a defect in insulin secretion or a defect in insulin action. If glucose is abnormally high in the blood for a long period of time, various complications arise due to chronic metabolic disturbance and subsequent chronic vascular injury. In this study, we tried to find natural substances with few side effects for the treatment of diabetic complications. Then, the chemical structure of the extract monomer was clarified and the synthesis of the final product was completed through 9 steps.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-302**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of dehydroascorbic acid derivatives with amine-based functional groups

Ju Hyun Song, Seongjoo Park, Dai Il Jung^{*}, JUNGTAI HAHN¹

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¹*Department of Beauty Care, UI University, Korea*

Dehydroascorbic acid is an oxidized form of ascorbic acid not be synthesized by humans, so it can be obtained by ingesting food and is actively introduced into the cell's vesicles through the glucose transporter. Ascorbic acid is not transmitted to the brain from the bloodstream, but the brain is one of the most common sources of ascorbic acid. Instead, dehydroascorbic acid is transported through the GLUT1 transporter through the blood brain barrier and then converted back to ascorbate. It can also protect nerve damage after ischemic stroke if administered as a medication. Drugs of amine type have drug effect. It is designed to mimic or interfere with the action of natural amine neurotransmitters. Therefore, the amine-based drugs are used as antidepressants and analgesics. However, it is severely addictive and has the risk of misuse and abuse. So in our laboratory we will synthesize dehydroascorbic acid derivatives with amine-based functional groups. Through these, fast delivery of nerves and brain is expected to have quick effects and few side effects.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-303**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Diversification of indazoles under transition metal catalyzed microwave reaction

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Department of Chemistry, Chungnam National University, Korea

¹*Korea Research Institute of Chemical Technology, Korea*

Indazoles, which are having pyrazole ring condensed with the benzene ring, are important class of heterocyclic compounds having a wide range of medicinal and biological properties. A number of derivatives of arylated indazole are known to possess potent pharmacological activity including anti-cancer, anti-bacteria, kinase inhibition. Therefore, the discovery of simple procedures allowing the easy access to arylated indazole derivatives is an important research area in organic chemistry. In this study, various substituted indazole derivatives have been synthesized by using Suzuki, Heck, and N-arylation coupling reactions with palladium and copper catalyst system under microwave irradiation.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-304**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Azeotropic drying-free aliphatic radiofluorination in mixed-organic solvent system

Young-Do Kwon, JEONGMIN SON¹, Mijin Yun, Joong-Hyun Chun *

Department of Nuclear Medicine, Yonsei University College of Medicine, Korea

¹*Department of Nuclear Medicine, Yonsei University Health System, Korea*

Positron emission tomography (PET) is a molecular imaging modality to study dynamics and metabolism associated with radiotracer distribution in living subjects. Widespread supply of cyclotron in hospitals facilitates this technology to diagnose various diseases at their early stage, which eventually benefits the overall patient care. Among many radionuclides produced from cyclotron, fluorine-18 is considered to be the radionuclide of a choice for providing the ideal imaging characteristics. Considering the short half-life ($t_{1/2} = 110$ min.) of fluorine-18, a short radiolabeling time is required in reliable radiofluorination method to introduce fluorine-18 onto the target molecule to afford the subsequent imaging studies. However, the hydration of [¹⁸F]fluoride ion is known to detrimental effect on the nucleophilicity of fluorine-18 itself, leading to poor overall labeling outcome. To overcome this hurdle, azeotropic-drying has been conventionally employed prior to radiofluorination, which is the tedious and time-consuming task. Herein, we introduced an efficient radiolabeling method without azeotropic drying process, by direct use of [¹⁸F]fluoride ion eluted from QMA with phase transfer catalyst. The eluted [¹⁸F]fluoride ion in acetonitrile was mixed with different organic solvents for radiofluorination, such as dimethyl sulfoxide and dimethyl formamide. The developed aliphatic radiofluorination methodology would allow the streamlined radiolabeling process, which eventually simplifies the overall radiopharmaceutical process specifically for clinical setting. This work was supported by the National Research Foundation (NRF) of Korea, funded by the Ministry of Science, ICT & Future Planning (NRF-2015R1D1A1A02061420).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-305**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Oxidized iodoarenes as versatile precursors for no-carrier-added (NCA) aromatic radiofluorination

Young-Do Kwon, JEONGMIN SON¹, Mijin Yun, Joong-Hyun Chun *

Department of Nuclear Medicine, Yonsei University College of Medicine, Korea

¹*Department of Nuclear Medicine, Yonsei University Health System, Korea*

Positron emission tomography (PET) is non-invasive imaging technology which allows monitoring distribution and concentration of radioligands *in vivo*. Many radiotracers developed for PET have been classically radiolabeled with cyclotron-produced carbon-11 and fluorine-18. Various fluorine-18 radiolabeling methodologies have been advanced by the widespread supply of cyclotrons in clinics. Unlike electrophilic methods, no-carrier-added nucleophilic radiofluorination with cyclotron-produced [¹⁸F]fluoride ion offers better molar radioactivity, which is an requirement to obtain quality PET images. Contrary to somewhat amenable aliphatic radiofluorination, the reliable aromatic [¹⁸F]fluorinations have not yet been established. Classified as λ^3 -organoiodines, among the polyvalent aryl iodine family, diaryliodonium salts and arylidonium ylides have been investigated as efficient precursors to give the corresponding [¹⁸F]fluoroarenes. Here, oxidized λ^3 -hypervalent aryl iodines were demonstrated as versatile precursors for fluorine-18 radiofluorination. We employed the convenient preparations of hypervalent iodoarene via simple oxidation of iodoarenes using readily-available oxidizing agents. The radiofluorination of λ^3 -hypervalent aryl iodine precursors proved to be a feasible single-step method for the radiosynthesis of useful [¹⁸F]fluoroarenes. This methodology would provide a useful means to prepare diverse [¹⁸F]fluoroarenes, which may be used to develop new fluorine-18 labeled radiotracers for PET imaging. This work was supported by the National Research Foundation (NRF) of Korea, funded by the Ministry of Science, ICT & Future Planning (NRF-2015R1D1A1A02061420).

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Code: **ORGN.P-306**

Area: Organic Chemistry

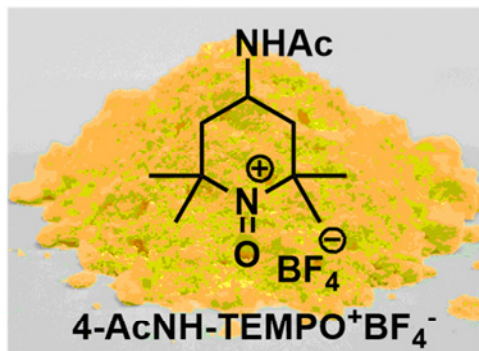
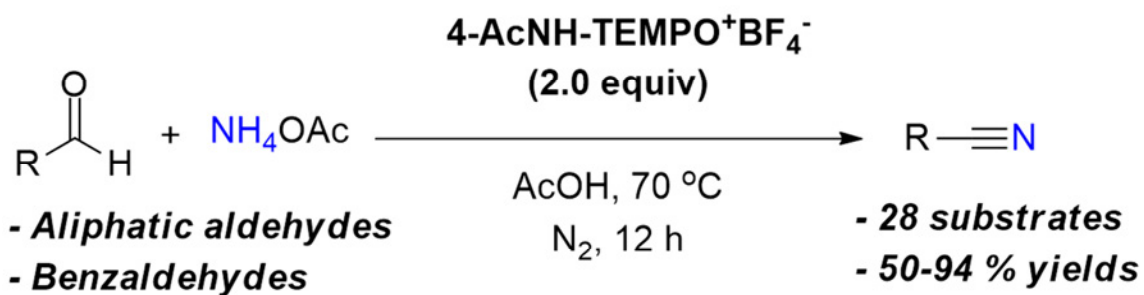
Type: Poster Presentation, Time: FRI 13:00~14:30

Oxoammonium Salt-Mediated Oxidative Nitriles Synthesis from Aldehydes with Ammonium Acetate

MYEONGJIN KIM, JINHO KIM*

Department of Chemistry, Incheon National University, Korea

Oxoammonium salts are interesting oxidants with three oxidation states; oxoammonium salts, nitroxyl radicals, and hydroxyl amines. The redox system between oxoammonium salts and hydroxyl amines is attractive because they are metal-free, less toxic, and recyclable. In addition, these systems provide highly selective oxidations under mild conditions. However, few examples of metal-free aldehydes to nitriles transformations mediated by oxoammonium salt were reported. Recently, our group achieved 4-acetamido-2,2,6,6-tetramethylpiperidine-N-oxyl (4-AcNH-TEMPO) catalyzed aerobic oxidative conversion of aldehydes to nitriles using easily available NH_4OAc . However, this catalytic system was not successful in the transformation of aliphatic aldehydes. Herein, we developed 4-AcNH-TEMPO⁺BF₄⁻-mediated nitriles synthesis from aliphatic as well as aromatic aldehydes with NH_4OAc .



- Readily accesible
- Selective
- Scalable
- Recyclable



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-307**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of photochromic polymers and study of its photochromic efficiency and fluorescence properties

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Department of Chemistry, Kyung Hee University, Korea

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Diarylethenes have been increasingly chosen as the preferred photochromic molecule due to their high fatigue resistance and thermal stability, which are essential prerequisites in many application including the manipulation of optical storage or switching devices. Control of fluorescence emission of diarylethenes has recently become important for some specific application, particularly the development of non-destructive readout memory and bio-imaging. We designed several photochromic monomers (PhBTT, BzBTT, PhBTTO4, BzBTTO4, etc.) and used them to synthesize polymers. PhBTT (BTT-Ph-CH₂=CH₂) was synthesized by Suzuki reaction and BzBTT (BTT-Bz-CH₂=CH₂) was synthesized by Friedel-Craft acylation reaction. In the case of the O4 series, oxidation was carried out using mCPBA. Then photochromic polymers were prepared using AIBN. The molecular weight is measured to check whether the polymer is produced. The polymer samples for the measurements were prepared as solutions and films. The absorption spectra and fluorescence were taken to confirm the photochromic-property of the polymer. The fatigue property of the polymer was also studied.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-308**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Coumarin Fluorescence Thiol Sensors Targeting Golgi Apparatus

Mijung Jang^{*}, Kihang Choi^{*}, Jeeun Lee

Department of Chemistry, Korea University, Korea

Golgi apparatus (GA) is a pivotal organelle for cell metabolism and participates in transporting and secreting proteins/enzymes. Glutaredoxin, one of the GA components, catalyzes the reduction of disulfide bonds in protein substrates using reduced glutathione (GSH) and, therefore, plays a key role in resisting oxidative stress. Thus GA is inevitably involved in redox process and can be considered as an important structure for the cellular antioxidant system. To study the role of GA in oxidative stress, we synthesized fluorescence probes which react with GSH inside GA of cancer cells. Cyclooxygenase-2 (COX-2) was chosen as a GA-specific target because it is overexpressed in virtually all cancer cell lines and accumulates significantly in GA. Indomethacin, a good inhibitor for COX-2, was used as GA-targeting moiety and linked to a coumarin fluorophore equipped with a thiol-reactive electrophile. We synthesized four probes with various linkers and test them with HeLa cell to ascertain the rise and fall of GSH levels in GA by monitoring fluorescence intensity changes. Our study shows that these fluorescence probes can be utilized successfully for the selective monitoring of GSH concentration changes in GA.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-309**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Hole transporting materials based on Spirobifluorene for OLEDs

Ji Hun Han, BRAVEENTH RAMANASKANDA, KIHUN YANG¹, Gyu Youn Chea*

Department of Chemistry, Wonkwang University, Korea

¹*School of Natural Science/Department of Chemistry, Wonkwang University, Korea*

Hole transporting materials based on Spiro compound (HTM 1A and HTM 1B) were synthesized by using Buchwald Hartwig and Suzuki cross coupling reaction with significant yields. Both the HTMs were exhibited higher decomposition temperature over 450 oC at 5% weight reduction and HTM 1B was revealed stable glass transition temperature of 180 oC. To understand the device properties, red phosphorescence based devices were fabricated by using HTM 1A and HTM 1B as hole transporting materials. Reference device was fabricated by using Spiro-NPB as hole transporting materials. HTM 1 B based device showed higher current and power efficiencies of 16.16 cd/A and 11.17 lm/W. Maximum external quantum efficiency (EQE) of HTM 1B based device was 13.64 % and which was higher than that of reference base device and HTM 1A.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-310**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Comparison of Coumarin Derivatives as Thiol Sensors Long-lasting inside Living cells

Mijung Jang^{*}, Kihang Choi^{*}

Department of Chemistry, Korea University, Korea

Thiol compounds play essential roles in biological system, and much attention has been paid to develop fluorescence sensors for biothiols. Most of the existing sensors are not suitable for continuous and selective monitoring of biothiols because these sensors react with the analytes in irreversible manners. For the bioimaging applications to study dynamic changes inside living systems, it is also required to develop fluorescence sensors long-lasting inside a cell. Here, we report the synthesis of coumarin derivatives which are expected to be long-lasting inside living cells. Fluorescence properties and cellular toxicities of these compounds are compared. These coumarin derivatives show thiol-concentration dependent bidirectional and reversible fluorescence changes through controlled experiment. Our study demonstrates that the newly developed fluorescence sensors can be used for the monitoring of thiol concentration changes over longer period of time.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-311**

Area: Organic Chemistry

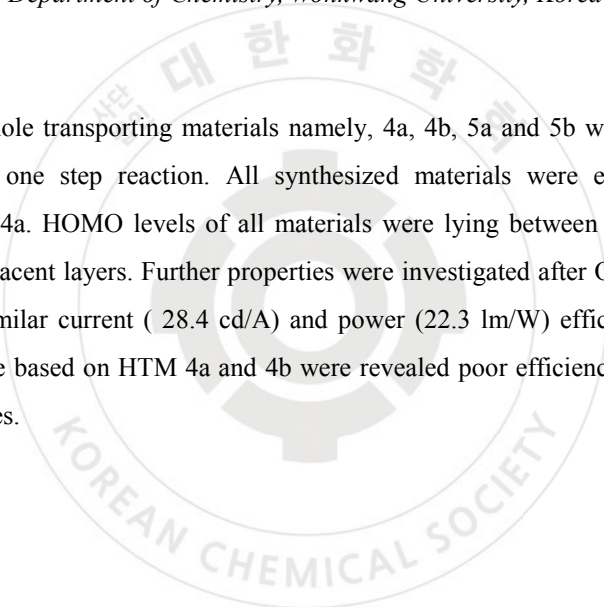
Type: Poster Presentation, Time: FRI 13:00~14:30

Triphenylamine based hole transporting materials for OLEDs

BRAVEENTH RAMANASKANDA, Ji Hun Han, Seon Guk, Gyu Youn Chea*

Department of Chemistry, Wonkwang University, Korea

Triphenylamine based hole transporting materials namely, 4a, 4b, 5a and 5b were synthesized by using Suzuki cross coupling one step reaction. All synthesized materials were exhibited higher thermal stabilities except HTM 4a. HOMO levels of all materials were lying between 5.38 eV to 5.44 eV and were match with the adjacent layers. Further properties were investigated after OLED device fabrication. HTM 5a was shown similar current (28.4 cd/A) and power (22.3 lm/W) efficiencies with NPB based reference device. Device based on HTM 4a and 4b were revealed poor efficiencies when compared with other HTM based devices.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-312**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Practical Direct Synthesis of Asymmetrical Ureas from Alloc-Protected Amine via Treatment of DABAL-Me₃

Hee-Kwon Kim

Department of Nuclear Medicine, Medical School, Chonbuk National University, Korea

Urea is one of the important chemical units found in a lot of natural products. Besides, various fields such as pharmaceuticals, polymers, dyes, and sensors have used urea structures. In many organic synthetic procedures, amine was usually protected by protecting group and utilized. Alloc group is commonly used protecting group for amine. Preparation of urea units from Alloc-protected amine usually consists of deprotection and reaction with the other amines. Thus, direct conversion of Alloc-protected amines into ureas is attractive in organic chemistry areas. Herein, facile synthetic method for the ureas from Alloc-protect amines is described. In the synthesis, Alloc-protect amines were treated with DABAL-Me₃ to give the desired ureas, and all transformations to ureas from Alloc-protected amines were accomplished in high yield. This result can provide potential application to the preparation of various asymmetrical ureas.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-313**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Characterization of New Donor-Acceptor Molecules Based on Phenothiazine and Quinoline

So Dam Kim, Tae Woo Kwon*

Department of Chemistry, Kyungsoong University, Korea

Phenyl phenothiazine has been used as electron donor component due to their low reversible oxidation potentials by virtue of the sulfur atom which can facilitate the hole transport of the carrier. Methyl or phenyl substituted quinolines are well known to be a good electron acceptor materials. In this study, we report the synthesis of 10-phenyl-2-(4-phenyl-3-(p-tolyl)quinolin-2-yl)-10H-phenothiazine, 2-(4-methyl-3-(p-tolyl)quinolin-2-yl)-10-phenyl-10H-phenothiazine, 2-(3,4-diphenylquinolin-2-yl)-10-phenyl-10H-phenothiazine, 2-(4-methyl-3-phenylquinolin-2-yl)-10-phenyl-10H-phenothiazine via Ullmann, Grignard, Friedlander reactions. Products were determined by using ¹H, ¹³C NMR, UV-Vis and Photoluminescence. Detailed synthetic routes and characterization of novel phenothiazine derivatives will be discussed.

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Code: **ORGN.P-314**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

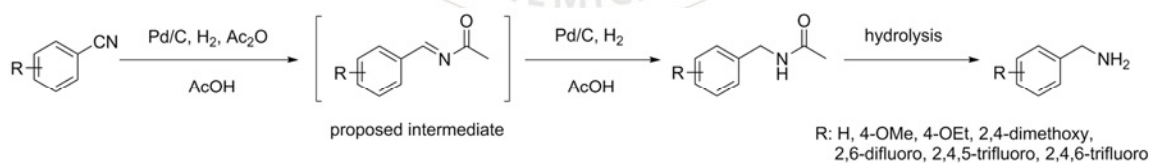
Facile and highly selective conversion of aromatic nitriles into primary amines

Junho Nam, Dong Guk Lee¹, KUN HOE CHUNG*

R&D part, Moghu research center, Korea

¹*College of Pharmacy, Korea University, Korea*

A number of studies have been conducted for decades to synthesize primary amines by catalytic hydrogenation of nitriles in various solvents. However, there is a drawback that unwanted secondary and tertiary amines are by-products of this reaction. In order to overcome this problem, a new experimental method was devised and the results obtained by this experiment are reported. The reaction of substituted benzonitriles, 5wt% Pd/C and acetic anhydride in acetic acid under hydrogen pressure gave corresponding acetamides in 86~99% yields. The desired amines are obtained by acid or base hydrolysis quantitatively.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-315**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemical and Photophysical Properties of Imidazole Fused Tetrathiafulvalene Derivatives

Ajeong Kim, Trang Thu Tran, Jung Su Park*

Department of Chemistry, Sookmyung Women's University, Korea

Fused electron donor-acceptor (D-A) systems have been attracted intensive research during the past few decades due to their potential applications including artificial photosynthetic systems, molecular electronics, or nonlinear optical materials. In an effort to develop an efficient D-A system, it has been reported that fusing electron-deficient nitrogen heterocycles to the TTF skeleton, for instance, quinoxaline, can increase the stability and charge mobility of the resultant organic D-A molecules.^[1] It was also reported that imidazole can enhance the electron-donating abilities of parent TTF skeleton.^[2] As such, we report here the synthesis and characterization of imidazole fused tetrathiafulvalene derivatives. These materials exhibit intramolecular charge transfer (ICT) band. Upon the protonation or Lewis acid-base complexation, largely red-shifted ICT bands were observed. The molecular structures were fully characterized by NMR, Mass-spectroscopic as well as X-ray crystallographic studies. The electrochemical and photophysical properties of these derivatives will be discussed in details based on UV-Vis, Fluorescence, EPR, and Cyclic Voltammetric studies.

References

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- [2] T. Murata, Y. Yamamoto, Y. Yakiyama, K. Nakasuji, Y. Morita, *Bull. Chem. Soc. Jpn.*, 2013, **86**, 927-939.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-316**

Area: Organic Chemistry

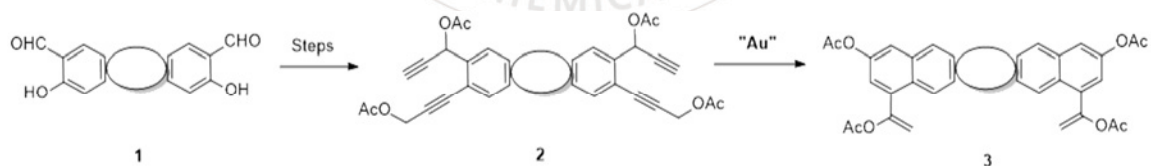
Type: Poster Presentation, Time: FRI 13:00~14:30

Dual Gold-Catalyzed Sequential Activation and proposed gold-carbene intermediate

JaeMun Jung, Min Sung Park, Chang Ho Oh^{*}, Jin Wook Han^{*}

Department of Chemistry, Hanyang University, Korea

Gold catalysis has emerged as an efficient methodology to activate π -systems of carbon-carbon double and triple bonds. The electrophilic π -system activation with alkenes, alkynes, and allenes toward for subsequent nucleophilic attack relies on electron deficiency of gold catalysts. We previously reported a novel Au-catalyzed sequential activation of two different propargyl carboxylates to 6-methylene-6H-benzo[7]annulene-5,8-diyl dicarboxylates. First, we will extended this reaction to prepare various substrates with 2 bearing double 1-(2-(3-acetoxyprop-1-ynyl)phenyl)prop-2-ynyl acetate and study their cyclization reactions under gold catalysts. Next, we proposed gold-carbene intermediate was supported by the control experiment for enyne metathesis route. we wish to report our preliminary results.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-317**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Intermolecular double aza Prins-type cyclization: A facile and efficient synthesis of 1,6-diazecanes

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¹*Chemoinformatics Research, Korea Institute of Science and Technology, Korea*

²*Department of Applied Chemistry, Hanyang University, Korea*

³*Korea Institute of Science and Technology, Korea*

Ten membered heterocyclic ring system containing nitrogen is a common structural feature of various natural products as well as designed functional organic molecules. It is difficult to find effective synthetic routes towards such compounds due to unfavourable entropic and enthalpic factors. The synthesis of these compounds is still very challenging. We have developed an efficient method to synthesize 1,6-diazecane derivatives by intermolecular double aza Prins-type cyclization of allenylmethylsilanes. The methodologies developed to obtain these compounds will be presented and discussed.

Conference Date: October 18~20, 2017

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Code: **ORGN.P-318**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Cyanine-Based Near-Infrared Fluorescent Probe for Nitroreductase

WON JOO LEE, Hae-Jo Kim *

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Hypoxia can cause an increase in reductive stress so nitroreductase (NTR) can be overexpressed in hypoxic tumors. Therefore, the detection of hypoxia and NTR is a feasible tool for the diagnosis of tumor cells and warrants robust detection for a biological study.^{1,2} A cyanine (Cy7) based dual optical probes were developed for detection of nitroreductase (NTR). Upon addition of NTR in the presence of NADH, the probe exhibited dramatic optical changes with strong fluorescence ($F/F_0 = 5.8$, $\lambda_{em} 748$ nm) as well as intense blue color ($\lambda_{abs} 650$ nm) by the nitro-to-amine functional group transformation and subsequent rearrangement in PBS buffer. The resulting colorimetric and fluorometric probe was successfully applied for the detection of mitochondrial NTR in vivo as well as in vitro.¹Xu, K.; Wang, F.; Pan, X.; Liu, R.; Ma, J.; Kong, F.; Tang, B. *Chem. Commun.*, **2013**, 49, 2554.² Li, Y.; Sun, Y.; Li, J.; Su, Q.; Yuan, W.; Dai, Y.; Han, C.; Wang, Q.; Feng, W.; Li, F. *J. Am. Chem. Soc.*, **2015**, 137, 6407.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-319**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Mitochondrial Targeting Oxazolidinoindole-Based Probe for Nitroreductase

HyunSeok Seo, Hae-Jo Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Biomedical studies indicate that the hypoxic status of solid tumors is closely related to the process of tumor progression. Therefore, the development of efficient methods for detecting the hypoxic conditions in living systems is very important for biomedical research. Nitroreductase is activated in a hypoxic condition such as cancer cells so the detection of hypoxia and NTR is a feasible tool for the diagnosis of tumor cells and warrants robust detection for a biological study.^{1,2,3,4,5} A fused oxazolidinoindole-based dual optical probe was developed for detection of nitroreductase (NTR). Upon addition of NTR in the presence of NADH, the probe exhibited dramatic optical changes with strong fluorescence ($F/F_0 = 14$, λ_{em} 580 nm) as well as intense orange color (λ_{abs} 460nm) by a nitro-to-amine functional group transformation and displayed a very low limit of detection (LOD = 10.4 ng/mL) of NTR in PBS buffer. Further application to endogenous cellular NTR was successfully applied in A549 cells, showing that the probe was clearly localized in a mitochondrial region.¹Padhani, A. R.; Krohn, K. A.; Lewis, J. S.; Alber, M. *Eur. Radiol*, **2007**, *17*, 861.²Brown, J. M.; William, W. R. *Nat. Rev. Cancer*, 2004, *4*, 437. ³Wilson, W. R.; Hay, M. P. *Nat. Rev. Cancer*, **2011**, *11*, 393.⁴Harris, A. L. *Nat. Rev. Cancer*, **2002**, *2*, 38 - 47.⁵Chen, Y.; Hu, L. *Med. Res. Rev*, **2009**, *29*, 29.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-320**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of α,α -dichloroketones from the reaction with alkyne and trichloroisocyanuric acid

Eunjeong Cho, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Dichloroketone can be transformed for the synthesis of biologically active heterocyclic compounds and good building block candidate. Classical methods using chlorinating reagents such as Cl_2 , sulfuryl chloride, ammonium salt of tetrachloridoiodate, $\text{SiCl}_4/\text{PhIO}$ and CuCl_2 required high temperature or harsh condition. Trichloroisocyanuric acid (TCCA) is known as chlorination reagent, inexpensive and stable. Recently, we found that trichloroacetophenone was formed when phenylpropionic acid was reacted with TCCA and H_2O . From this result, we envisioned that TCCA might afford α,α -dichloroketone from the reaction with diarylalkyne. As a much more efficient and convenient method, we developed the synthesis of dichloroketone by using the sequential reactions of coupling and chlorination. Arylbromide and propionic acid were allowed to react in the presence of 5 mol% $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$, 10 mol% dppb and 2.0 equivalent of DBU. The mixture was allowed to react with TCCA in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$. The reactions with diarylalkyne and TCCA afforded the desired α,α -dichloroketones in moderate to good yields. In addition, they all were obtained from the sequential reaction of decarboxylative coupling and chlorination. This chlorination was conducted at room temperature and showed good tolerance toward functional groups such as chloride, bromide, aldehyde and ketone.

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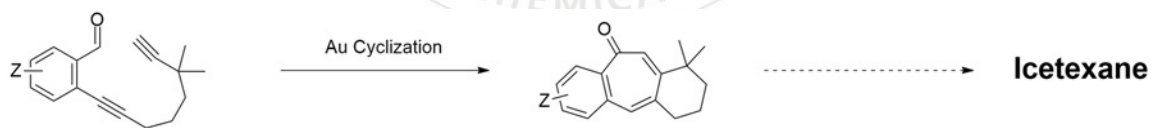
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Taxamairin B: Use of Au-Catalyzed Cyclization Reaction

Seonmi Lee

Department of Chemistry, Hanyang University, Korea

The 6-7-6 tricyclic diterpenoids, a rare structural type of diterpene thought to arise from the rearrangement of the more familiar abietane skeleton, has received considerable attention in the last few years for their structural features and biological properties. Among them, Taxamairin A and B have been isolated from the bark of *Taxus mairei* in 1987. An initial survey of Taxamairin A and B identified inhibitory activity against hepatoma (liver tumor) cells.¹ We have developed metal catalyzed cycloisomerization and hydrative cyclization reaction for construction of polycyclic ring systems with rhodium, platinum and gold catalyst. The Taxamairin B has been synthesized by a facile route, which employed the Au-catalyzed cyclization of an enynal that was easily prepared in a convergent manner. References [1] E. M. Simmons and R. Sarpong, *Nat. Prod. Rep.* 2009, 26, 1195–1217



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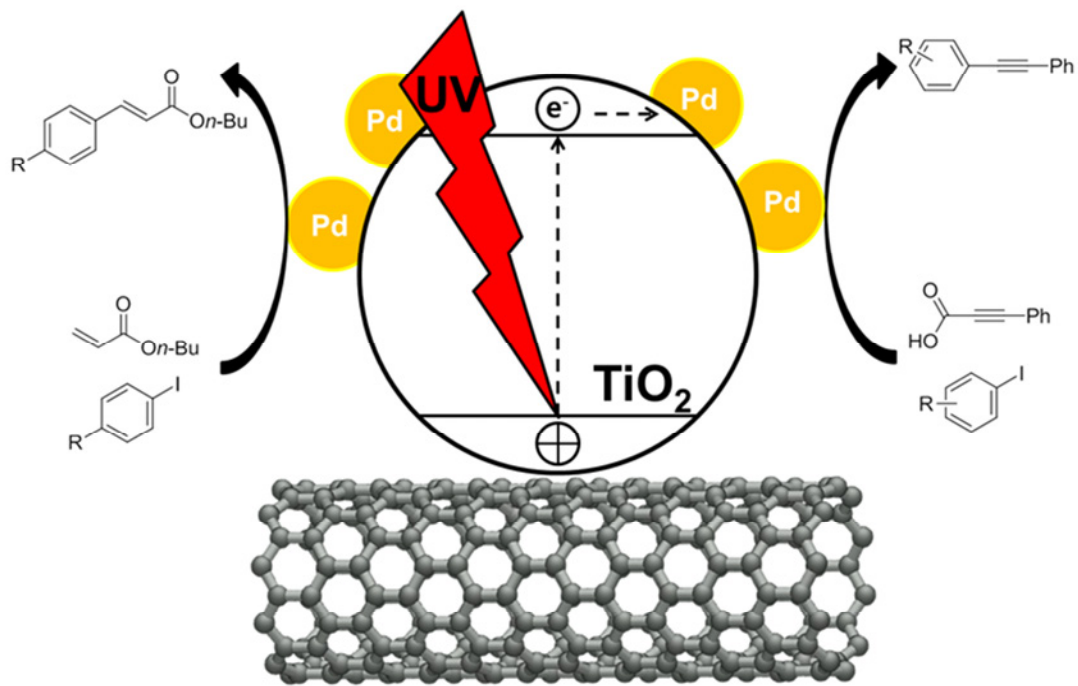
Type: Poster Presentation, Time: FRI 13:00~14:30

UV-Irradiation-Mediated Pd-Nanoparticle Catalytic System for the Heck and Decarboxylative Coupling Reactions

Han-Sung Kim, Jidang Kim, Hyun Chul Choi*, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

This study has been undertaken to investigate the UV irradiation effect on catalytic activities in Pd-catalyzed cross coupling reactions. A Pd-TiO₂-CNT composite was prepared by a previously reported sol-gel method, whereby anatase TiO₂ and metallic palladium nanoparticles were deposited onto the surface of carbon nanotubes (CNTs). The average particle size of these nanoparticles was determined to be ~4.3 nm by transmission electron microscopy. The prepared Pd-TiO₂-CNT material was employed as a catalyst for the Heck and decarboxylative coupling reactions, and it showed higher catalytic activity in the presence of UV irradiation than in the absence of UV irradiation. The enhanced catalytic activity of this system can be explained by the increased nucleophilicity of Pd due to electron transfer from TiO₂ under UV irradiation.



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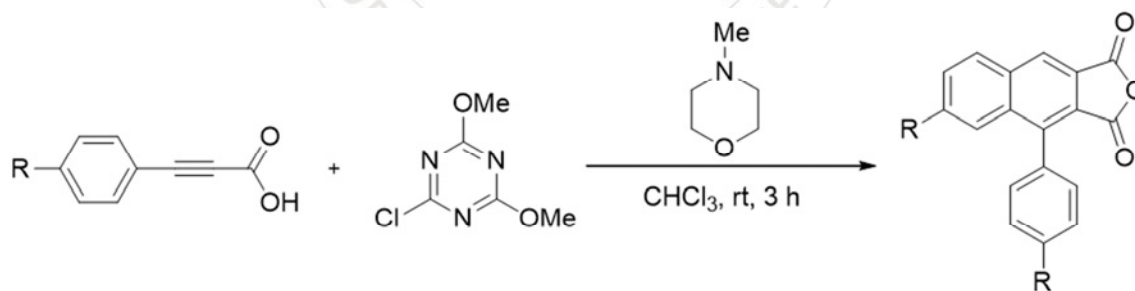
Type: Poster Presentation, Time: FRI 13:00~14:30

Room temperature cyclization of arylpropionic acid anhydride: Synthesis of naphtho[2,3-c]furan-1,3-dione derivatives

Jaerim Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Naphtho[2,3-c]furan-1,3-dione derivatives have received significant attention from pharmaceutical and material scientists owing to the fact that they have contributed to the synthesis of some very useful functional compounds. In the study of the decarboxylative coupling reaction of phenylpropionic acid, we found that the reaction with 2-chloro-4,6-dimethoxy-1,3,5-triazine (CDMT) provided 4-phenyl naphtho[2,3c]furan-1,3-dione at room temperature. It is known that CDMT is stable and inexpensive. This motivated us to develop a mild synthetic method of naphtho [2,3-c]furan-1,3-dione derivatives.



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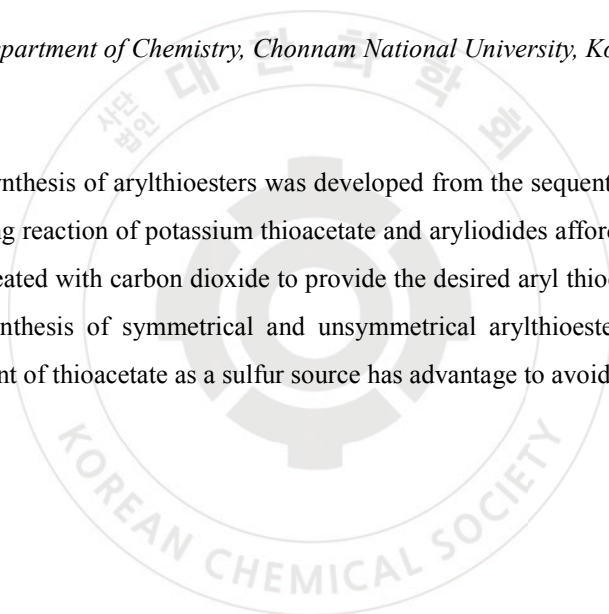
Type: Poster Presentation, Time: FRI 13:00~14:30

Pd-Catalyzed One-Pot Synthesis of Arylthioesters via C-S Coupling and Carbonylation

Myungjin Kim, Sunwoo Lee^{*}

Department of Chemistry, Chonnam National University, Korea

Pd-catalyzed one-pot synthesis of arylthioesters was developed from the sequential reaction of potassium thioacetate. The coupling reaction of potassium thioacetate and aryl iodides afforded aryl thioacetate. This reaction mixture was treated with carbon dioxide to provide the desired aryl thioesters. This methodology enables the one-pot synthesis of symmetrical and unsymmetrical arylthioesters with good yields. In addition, the employment of thioacetate as a sulfur source has advantage to avoid fetid odor.



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Palladium Catalyzed Decarboxylative Coupling of Aryl Chlorides with Alkynyl Carboxylic Acids

juhyeon Lee, Sunwoo Lee^{*}

Department of Chemistry, Chonnam National University, Korea

Aryl iodides, bromides, and chlorides have been employed as coupling partners of terminal alkynes. Among these, aryl iodides are the most reactive substrate, aryl bromides have intermediate reactivity, and aryl chlorides are relatively inert electrophiles. However, aryl chlorides have the advantages of being available and inexpensive. Therefore, several methodologies for Sonogashira coupling reactions employing aryl chlorides have been developed. Very recently, we developed palladium-catalyzed decarboxylative coupling reactions with aryl tosylates, which are known as the least reactive electrophiles in coupling reactions. This success prompted us to develop decarboxylative coupling reactions using aryl chloride. Aryl chlorides were employed as coupling partners in the decarboxylative coupling reactions of propiolic acid derivatives. The optimized conditions were found to involve the use of Pd(OAc)₂ and Josiphos in the presence of Cs₂CO₃ in DMSO. The desired coupled products were obtained in moderate to good yields.

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PdPt-Fe₃O₄-Catalyzed C-H Silylation Reaction of Aryl Halide with Triethylsilane

jisun jang, Byeong Moon Kim^{1,*}, Sunwoo Lee^{*}

Department of Chemistry, Chonnam National University, Korea

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

Arylsilanes are very valuable synthetic building blocks in pharmaceutical and material chemistry due to their unique properties. Classically, silyl groups have been introduced by using the reaction with lithium or Grignard reagents and silicon electrophile, however, this method lack the functional group tolerance toward base-sensitive group. As an alternative method, transition metal-catalyzed coupling reactions with aryl halide with disilanes or hydrosilane have widely been used. Recently, the direct C-H silylation has received much attention as attractive alternative because it is the most powerful and atom-economical tool. However, they can be used to the limited substrates such as heteroarenes and arenes bearing ortho-directing group. Generally, transition-metal catalyzed silylations from aryl halides or C-H activation were all homogeneous catalysis, but reusable catalytic system has never been developed in silylation. Bimetallic catalysis has received much attention for the synthesis of target molecules which are unattainable by using conventional monometallic catalyst. Very recently, we developed bimetallic Pd-Pt-Fe₃O₄ nanoflake-shaped alloy nanoparticle and employed as a catalyst for reduction of nitroarenes. This magnetically recoverable nanoparticle provided nearly quantitative conversions and yields, and reused up to 250 times. It has been reported that bimetallic nanoparticle showed extraordinary catalytic activities that are better than those of the parent metals. We envisioned that bimetallic Pd-Pt-Fe₃O₄ catalyst exhibits better activity than single metal catalytic system in the silylation. We found some drawbacks in palladium or platinum-catalyzed silylation. The former case required specific phosphine ligand which is unstable or expensive, and the latter case needed expensive platinum even though ligand was not required. Therefore, the employment of Pd-Pt-Fe₃O₄ as catalyst is expected to address these issues, and furthermore, it provide reusable and easy recoverable catalytic system.



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Paper-Based Colorimetric ChemoSensor for Halide ion High-Throughput Screening of the Coupling Reactions

Yujeong Son, Min Sik Eom¹, Min Su Han^{1,*}, Sunwoo Lee^{*}

Department of Chemistry, Chonnam National University, Korea

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

Because of the demand for the fast analysis of reaction leads to synthetic methodology development, several high-throughput screening(HTS) methods have been developed. We previously reported colorimetric analysis methods of the sensor for detection of halide ion using mercury complex of 4-(2-pyridylazo)resorcinol(PAR-2Hg⁺) by UV/vis spectroscopy correlated well. We can expand PAR-2Hg⁺ complex from solution type sensor to paper based sensor. This paper-based chemosensor exhibited a high selectivity for halide ions because the complex converted to free PAR in the presence of halide ions to be binding to Hg⁺ of the complex. We easily obtained information of conversion the reactions from the colorimetric change in the reactions without any equipment.

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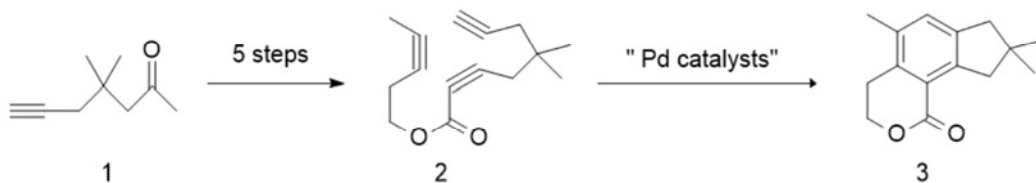
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Alcyopterosin series via Palladium Catalyzed Cyclization of triynes

Juyeon Kang

Department of Chemistry, Hanyang University, Korea

Synthesis of polycyclic compound has been a major challenge in modern synthetic organic chemistry due to the large appearance of biologically active natural products possessing polycyclic rings. Triynes can be converted into polycyclic compounds with the help of the transition metal catalysts like palladium, rhodium, nickel, and cobalt. Continuing our interest in palladium catalyzed polycyclization, we revisited [2+2+2] triyne cyclization to synthesize the Alcyopterosin natural products. We will report the synthesis of some of Alcyopterosin Natural products starting from the enone L.



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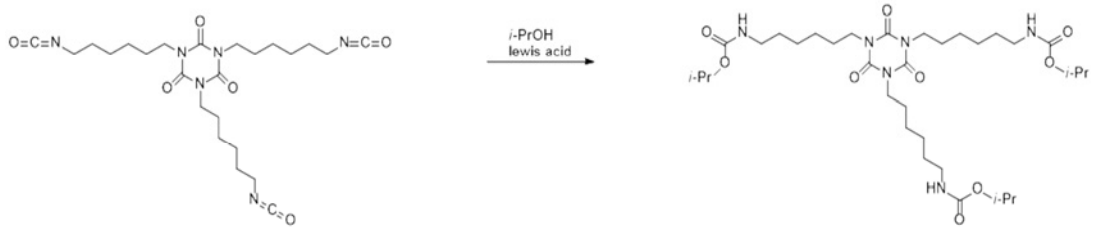
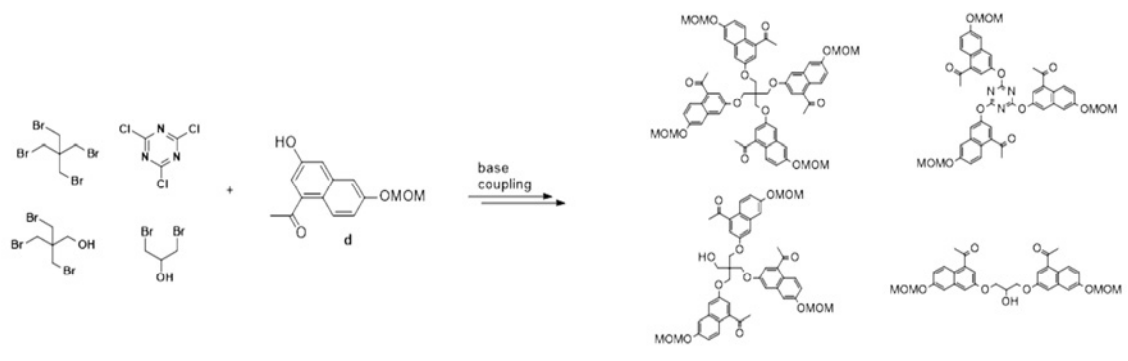
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Dendrimer Type Systems via Alcohol Coupling with Haloalkyl and Isocyanate Compounds under Basic and Acidic Conditions

Jaewoong Kim, Kun Hee Kim, Chang Ho Oh^{*}, Jin Wook Han^{*}

Department of Chemistry, Hanyang University, Korea

Jaewoong Kim, Kun Hee Kim, Chang Ho Oh^{*}, Jin Wook Han^{*} Department of Chemistry, Hanyang University, Wangsimni-ro 222, Seongdonggu, Seoul 04763, Korea Au-catalyzed [4+2] cycloaddition of two propargylic carboxylate was developed by our lab. Naphthyl compound **c** was synthesized via this gold reaction. To extend this **c** for multi naphthyl compounds, naphthyl alcohol **d** was applied for dendron concept. This acidic alcohol was well multi-coupled with cyanuric chloride and aliphatic bromoalkyl compounds under base. And also we developed the condition of non-acidic alcohol coupling for further reaction. Isopropyl alcohol (secondary alcohol) was multi-coupled with isocyanate group under lewis acidic condition successfully. In short, we synthesized a series of multi arms compounds via alcohol-coupling with haloalkyl and isocyanate compounds under basic and acidic condition.



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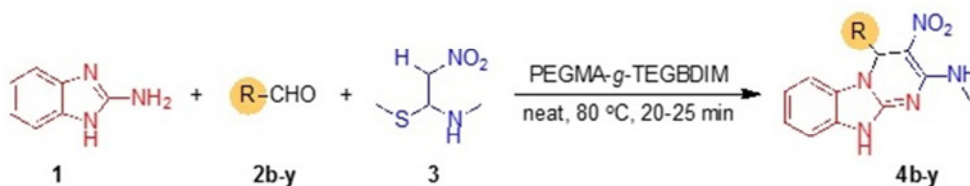
Polymer Supported Ionic Liquid as an efficient and recyclable catalyst for the Synthesis of benzo[4,5]imidazo[1,2-a]pyrimidines

Veeranarayana Reddy Mudumala, KANG ROK BYEON, SEOKMIN KANG, Dong Wook

Kim *

Department of Chemistry, Inha University, Korea

An efficient, highly active and reusable polyethylene glycol methacrylate-grafted tetra-ethylene glycol-bridged dicationic imidazolium-based ionic liquid (PEGMA-g-TEGBDIM) catalysed a regioselective cascade synthesis of benzo[4,5]imidazo[1,2-a]pyrimidines via multicomponent reactions of 1H-benzo[d]imidazol-2-amine, aldehydes and (E)-N-methyl-1-(methylthio)-2-nitroethenamine under solvent-free conditions. This protocol perfectly obeys the features of green chemistry, including having no waste regarding side-products, being solvent-free; having free from column chromatographic purification and a recyclable catalyst are the important features of this protocol.



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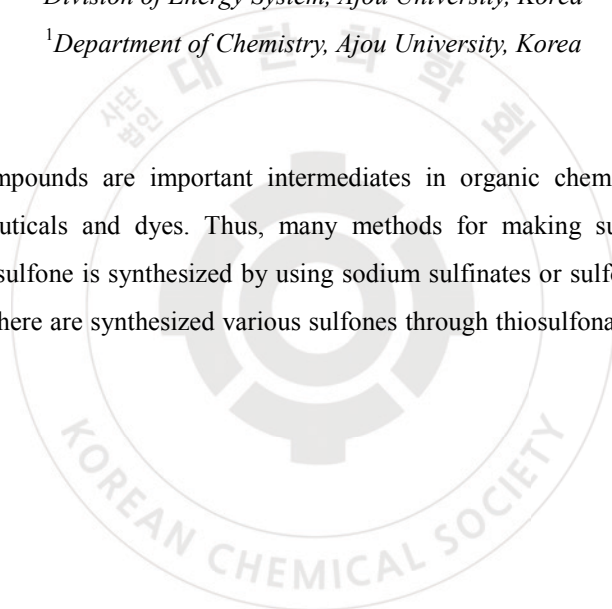
Synthesis of Various Sulfone via Thiosulfonates

Sang Joon Hwang, Hye-Young Jang^{1,*}

Division of Energy System, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Sulfone-containing compounds are important intermediates in organic chemistry, as well as in the synthesis of pharmaceuticals and dyes. Thus, many methods for making sulfone bonds have been developed. In general, sulfone is synthesized by using sodium sulfinates or sulfonyl chlorides as sulfone sources. In this study, there are synthesized various sulfones through thiosulfonates which easy to handle it.



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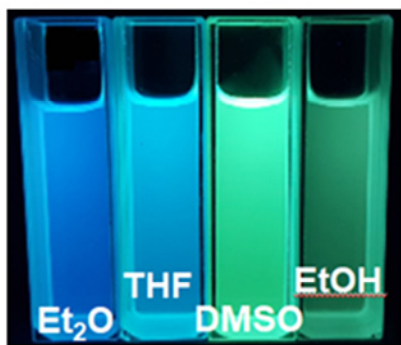
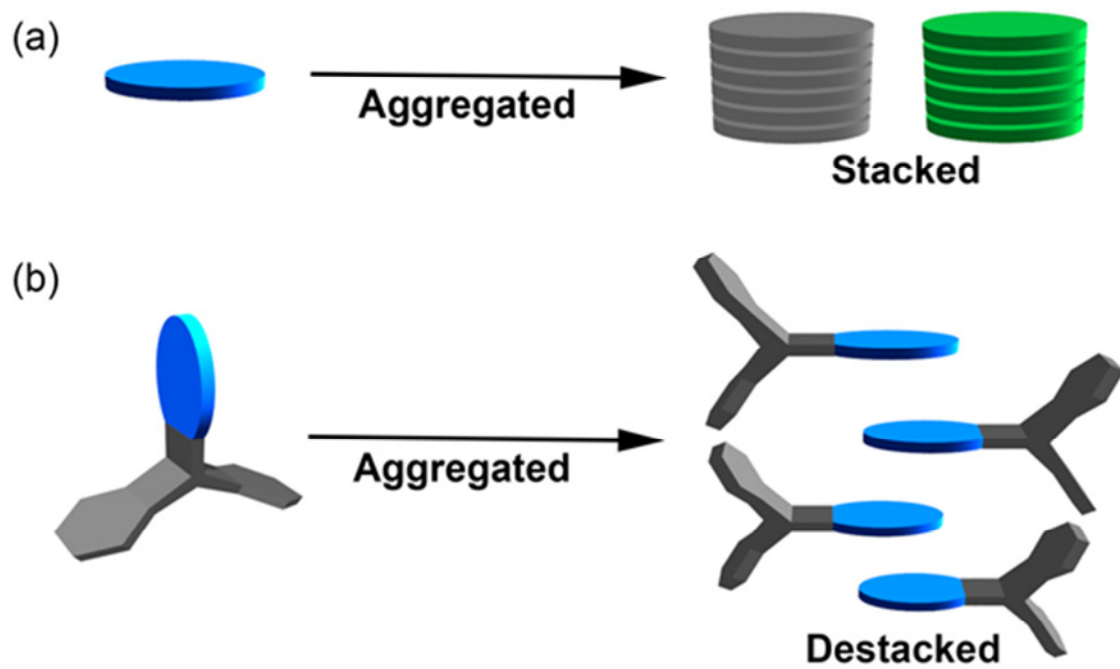
Type: Poster Presentation, Time: FRI 13:00~14:30

Triazoliptycenes: Stereoelectronic Control of Molecular Fluorescence and Solid-State Self-Assembly

Taewon Kang, Hongsik Kim, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Photophysical properties of small molecules can be controlled by modifying chemical structures. In the condensed phase, however, molecular fluorescence often deviates significantly from that of discrete species in solution. To address this problem, we have devised and implemented an intuitive steric model to control crystal packing and intermolecular interactions. Specifically, triazole-based fluorophores were integrated into the iptycene scaffold that suppresses close π - π contacts in the solid state. As it turned out, a stereoelectronic bias imposed by the iptycene scaffold allowed for regioselective C-N cross coupling as the key step in the modular synthesis. A combination of experimental and computational studies established the dual role of the iptycene motif as a π - π de-stacker and regio-controller group in synthesis. Both properties were deliberately exploited to build a new class of non-stacking organic fluorophores having tunable spectral windows.



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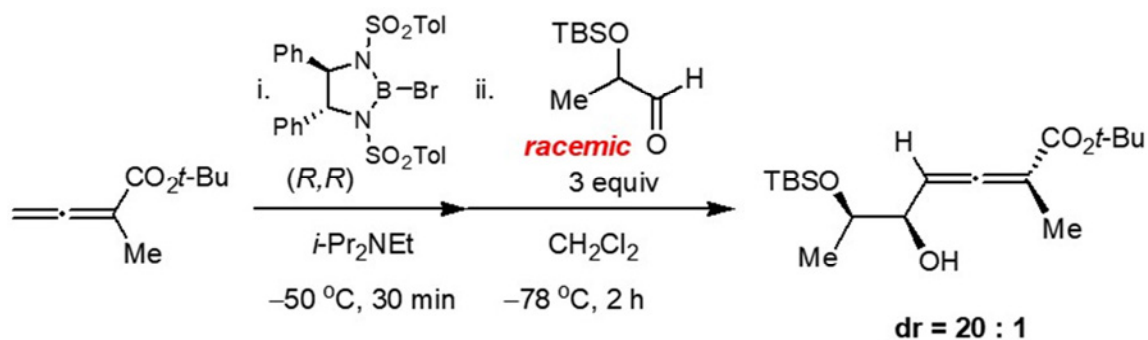
A Highly Efficient Kinetic Resolution of Racemic Aldehydes in Carbonyl Addition Reaction of 1-Alkylallenoates in Forming Gamma Adducts

hee jung jeong, Changhwa Oh, Jieun Lee¹, JIMIN KIM^{*}, Chan-Mo Yu^{1,*}

Department of Chemistry, Chonnam National University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

The availability of efficient synthetic methods for achieving absolute stereoselectivity in the production of enantiomerically pure compounds is of considerable current interest because such products can be used as chiral building blocks for the synthesis of valuable chiral molecules. Recently, we discovered a highly stereoselective synthesis of unusual gamma aldol adducts from the reaction of allyl-alkyl allenoate with a chiral bromoborane in the presence of *i*Pr₂NEt, and then aldehydes. The characteristic features of our approaches in terms of structural aspects of the products have encouraged us to carry out more investigations for designing new asymmetric routes using allenylsubstrates. We present herein our discovery of control elements to regulate diastereoselective formation of a gamma adduct from the reaction of 1-alkylallenoates with racemic aldehydes through a kinetic resolution, which allows in good yields with high levels of stereoselectivity as describe below. We would like to present herein scope and limitation of the reaction and its synthetic applications to natural products.



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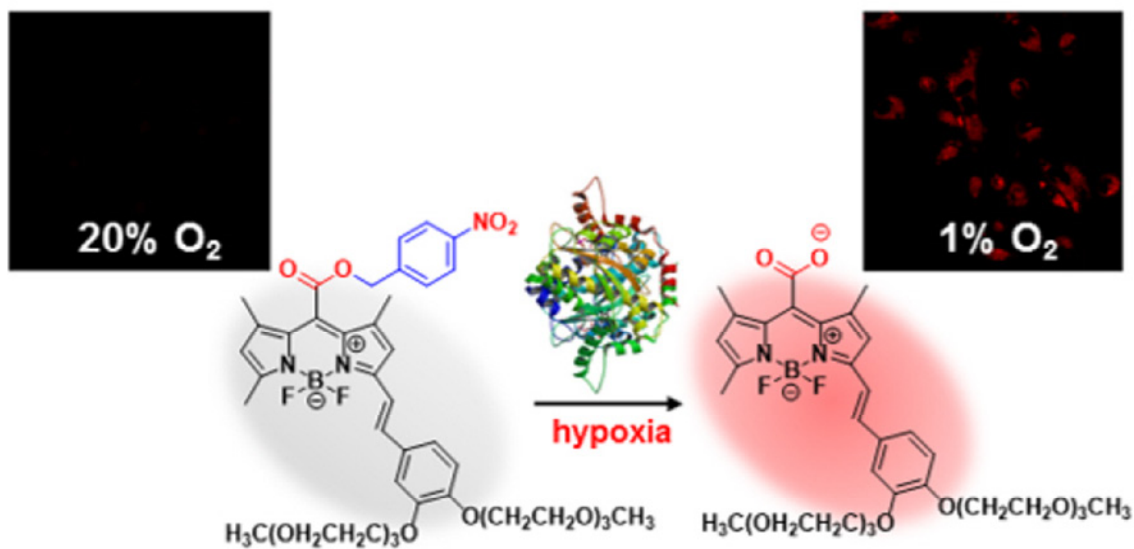
***meso*-ester BODIPYs for the imaging of hypoxia in tumor cells**

TEAIL KIM, youngmi kim^{1,*}

Kyung Hee University, Korea

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

Recently we have reported that the photophysical properties of *meso*-substituted-1,3,5,7-tetramethyl-BODIPY dyes rely on the electronic and steric effects of the *meso*-substituents.¹ In particular, the conversion of a *meso*-ester group to the corresponding *meso*-carboxylate of 1,3,5,7-tetramethyl-BODIPY dyes leads to the remarkable enhancement in fluorescence emission. By taking advantage of this feature, we developed the *p*-nitrobenzyl ester of a *meso*-carboxyl BODIPY as a new fluorogenic probe for the monitoring of nitroreductase, which catalyzes reduction of the nitroaromatic substrates to the corresponding amino one in hypoxic cancer cells. The probe exhibits weak fluorescence emission in far-red region in aqueous buffer solution, but upon incubation of probe with nitroreductase, absorption and fluorescence emission profiles are blue-shifted with significantly enhanced fluorescence intensity (~220-fold), indicating that highly fluorescent *meso*-carboxylate BODIPY dye was formed from the reduction of the *p*-nitrobenzyl group in probe to the corresponding *p*-aminobenzyl derivative, and subsequently 1,6-elimination reaction of *p*-azaquinone methide. The probe also showed high sensitivity (detection limit of 0.9 ng/mL), and high selectivity for nitroreductase over other biorelated species. In vitro cell studies confirmed its utility for the rapid fluorescence imaging of hypoxic cancer cells.¹Reference1. (a) Kim, S.; Bouffard, J.; Kim, Y. *Chem. Eur. J.* 2015, 21, 17459–17465. (b) Kim, S.; Kim, H.; Choi, Y.; Kim, Y. *Chem. Eur. J.* 2015, 21, 9645–9649. 2. Kim, T.-I.; Kim, H.; Choi, Y.; Kim, Y. *Sens. Actuators B. Chemical* 2017, 249, 229–234.



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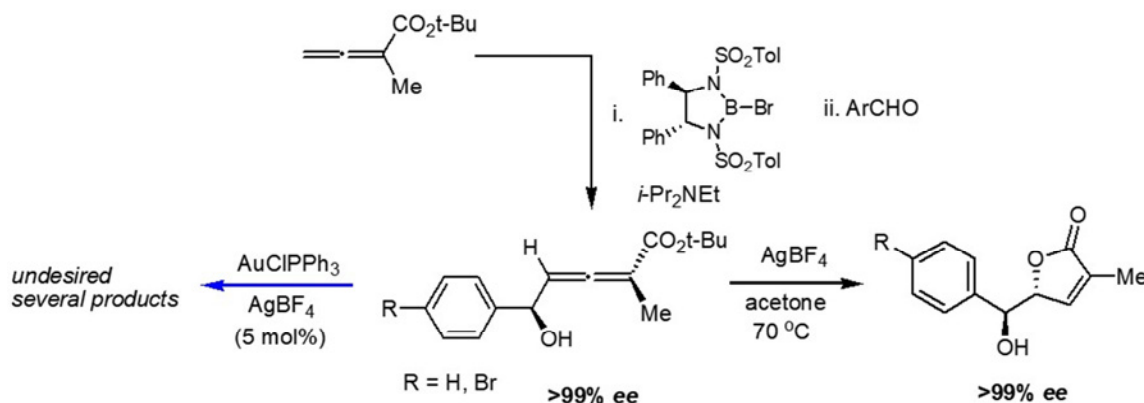
A Regiospecific Oxacyclization of 5-Aryl-5-hydroxy-2,3-allenoates Using Ag(I) in Acetone

SAEHANSAEM PARK, Jieun Lee¹, Changhwa Oh, Chan-Mo Yu^{1,*}, JIMIN KIM^{*}

Department of Chemistry, Chonnam National University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

The availability of efficient synthetic methods in the construction of cyclic systems via organotransition metal catalysts is of considerable current interest in organic chemistry. In this regard, an allene has been proven to be a useful substrate for a variety of transition metal catalytic reactions, particularly for the cyclizations in the construction of carbo- and heterocycles. As part of our investigations utilizing allenoates as versatile substrates for asymmetric carbonyl additions, we have developed new synthetic methods for the synthesis of 5-hydroxy-2,3-allenoate in regio- and stereospecific manner from the reaction of 1-alkyl allenoate and chiral bromoborane with aldehydes. As a part of an application, a regiospecific cyclization of 5-hydroxy-2,3-dienoates via gold catalysis was demonstrated. Although 5-alkyl gamma adducts proved to be effective, 5-aryl gamma adducts exhibited problematic for the gold cyclization. After surveying numerous conditions, Ag(I) in acetone at 70 °C could be a proper conditions. We will present scope and limitation of the oxacyclization.



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Total Synthesis of Isohericenone via Cu-Catalyzed Methylboration of Functionalized Terminal Alkyne

Yunmi Lee^{*}, yuna kim

Department of Chemistry, Kwangwoon University, Korea

Isohericenone was isolated from *Hericium erinaceum*, which is an edible mushroom and has been used in traditional Chinese medicine. In recent years, its inhibitory activity against various human cancer cells was evaluated and the biological results suggested that isohericenone could be studied as potential targets for anticancer drug discovery. Therefore, an efficient synthetic approach to isohericenone is needed. Herein, we described an efficient and concise total synthesis of isohericenone through three key steps: Mannich reaction with commercially available hydroxybenzoate to synthesize the isoindolinone core structure, Cu-catalyzed methylboration of terminal alkyne to afford the C5'-oxidized geranyl side chain, and Suzuki-Miyaura reaction to couple the geranyl unit with the isoindolinone core.

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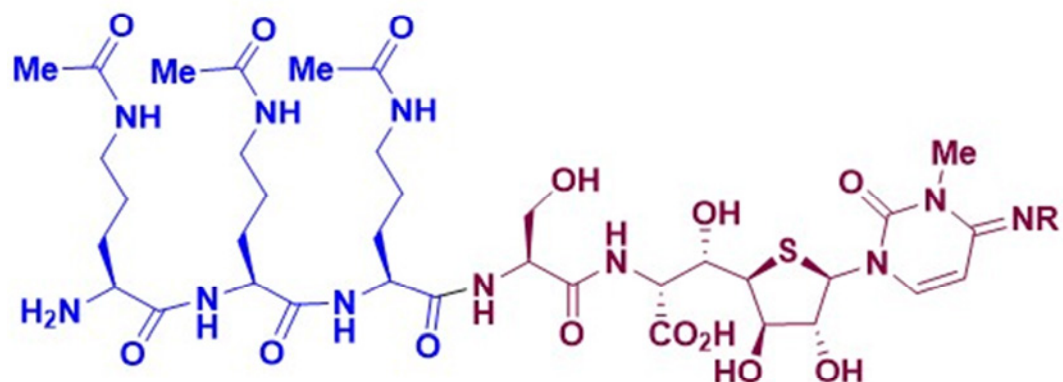
Studies towards elucidation of the biosynthetic mechanism of a natural product sideromycin, albomycin δ_2

yeasong park, jinhyo hwang, Woon Young SONG, Na lee Kim, Hak Joong Kim*

Department of Chemistry, Korea University, Korea

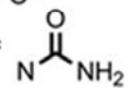
Bacteria emit a substance called "sideromycin" when another competing bacterium against ferric ion. Sideromycin is a form in which antibiotics are conjugated siderophore. This sideromycin can kill other bacteria and act as siderophore for itself. This strategy is called "Trojan horse". Typical examples of sideromycin are "albomycin" and "salmycin". We aim to study the natural product, albomycin, as a target. Albomycin is a natural product extracted from streptomyces sp. Its antibiotic effect in vivo and in vitro is known to be very good. The structure of the albomycin is linked to the ferrichrome part(siderophore) and the antimicrobial part, SB-217452, by a peptide bond. SB-217452 has a thionucleoside moiety and three different types, ϵ , δ_1 , and δ_2 . When the albomycin enters another bacterium, the siderophore and the antibiotic part are split into two parts, and the antibiotic part is attached to the serine t-RNA synthetase. This resembles serine-AMP (serine-adenosine monophosphate) and interferes the action of t-RNA synthetase. Although total synthesis of ϵ and δ_1 is reported, the yield is very poor, and Synthesis of δ_2 hasn't been reported. The biosynthetic pathway is also not fully understood. Therefore, it is necessary not only to synthesize the moiety of SB-217452 of δ_2 , but also to clarify biosynthetic pathway.

Ferrichrome



Albomycin ϵ R = NH

Albomycin δ_1 R = O

Albomycin δ_2 R = 



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Synthesis and Photochromic Behavior of Spiropyran-Triazine

Go-Eun Choi, Eun Ju Shin*

Department of Chemistry, Suncheon National University, Korea

In the recent years, there has been considerable interest in the design of artificial molecular probes for recognition and quantification of metal ions. Spiropyrans are attractive platforms in such constructions due to their unique photochromic property and molecular recognition ability. The electrically neutral spiropyran undergoes isomerization from its spiropyran form to the corresponding zwitterionic trans-merocyanine form. Their switchability is due to reversible heterolytic cleavage of the spiro C–O bond upon UV irradiation, followed by cis–trans isomerization by UV-vis irradiation and vice-versa by visible light irradiation. The negatively charged phenolic oxygen in the zwitterionic open form also produces a moiety that can convert the neutral spiropyran into an efficient ligand for protons and metal ions. A new spiropyran derivative containing triazine moiety was designed and synthesized. Photochromic behavior of spiropyran-triazine has been investigated by ultraviolet-visible absorption and fluorescence spectroscopic measurements.

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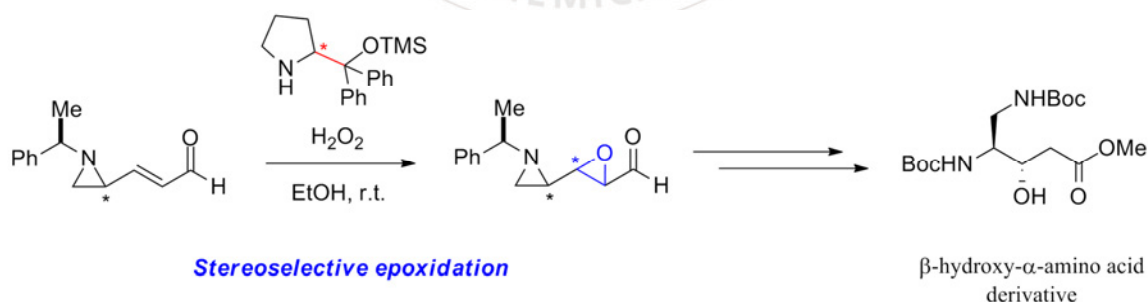
Organocatalyzed asymmetric epoxidation of aziridin-2-ylacrylaldehyde : Synthesis of β -hydroxy- α -amino acid derivative

Hyeonsu Jeong, Hyun-Joon Ha^{*}, Jung Woon Yang^{1,*}

Department of Chemistry, Hankuk University of Foreign Studies, Korea

¹*Department of Energy Science, Sungkyunkwan University, Korea*

(*R*)-phenylethyl aziridine-2-ylloxirane-2-carbaldehyde bearing both of aziridine and oxirane functional groups in a single molecule was prepared from aziridine-2-yl-acrylaldehyde through stereoselective epoxidation with organocatalyst. Chemical and regiospecific ring-opening either at aziridine or at oxirane were successfully achieved. In the presence of NHC catalyst and alcohol, oxirane was converted to alkyl 3-(aziridin-2-yl)-3-hydroxypropionate in high yields which allowed us to determine the stereochemistry of epoxy aziridine. On the basis of this reaction, β -hydroxy- α -amino acid derivative was also achieved in 70% overall yield.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-340**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Photoinduced Proton Dissociation of Merocyanine-sulfonate Photoacid

Go-Eun Choi, Eun Ju Shin*

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Over the past years, merocyanine-sulfonate type photoacid in controlling proton transfer in chemical, material and biological processes have been reported. Sulfonate-functionalized merocyanine photoacid (MEH) undergoes a cyclization reaction under visible light to form a protonated spiropyran (SPH), which is highly acidic. Protonated spiropyran (SPH) releases a proton to form a spiropyran. For the applications under aqueous conditions, stability of this type of photoacid has been a concern. In addition, protonated spiropyran as a relatively strong acid is expected to be applicable to various acid-catalyzed chemical reactions. In this study, photoinduced proton transfer process of merocyanine-sulfonate type photoacid has been investigated by using UV-vis absorption and fluorescence spectroscopic measurements.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Rhodamine-Spiropyran Fe(III)-Selective Chemosensor via Color Changes and Fluorescence Enhancement

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Department of Chemistry, Suncheon National University, Korea

Among the probes developed, the rhodamine(Rh)-based fluorescent probes have already attracted great interest due to the valuable characteristics of rhodamine derivatives, such as high molar extinction coefficient, large fluorescence quantum yield and a unique ring-opening process with turn-on signals. In addition, rhodamine-based compounds are ideal candidates for fluorescent sensors because of their good photophysical properties, such as absorption and emission wavelengths elongated to the visible region, high fluorescence quantum yield, and large absorption coefficient. Spiropyran(SP) derivatives are one of the most widely studied classes of photoswitchable compounds, whose molecular structure can be altered after exposure to light, temperature, pH or electrochemistry. They would undergo reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range. As one of the essential trace elements in biological systems, Fe³⁺ plays a crucial role in living organisms and metabolism. For example, it is an essential element for the formation of the hemoglobin of vertebrate red cells and plays a vital role in the storage and transport of oxygen to tissues. However, iron level should be balanced in human being. Excessive Fe³⁺ in the human body has been found to be related to an increased incidence of certain cancers and the dysfunction of certain organs, with symptoms such as diarrhea, vomiting, stomach pain, and heart/liver damage. Therefore, the simple and fast detection and separation of iron ions are very desirable. For the detection of Fe³⁺, fluorescent sensors are especially attractive due to their advantages such as high sensitivity, noninvasiveness, and convenience. In this work, rhodamine-spiropyran dyad has been prepared and investigated its ability as a Fe³⁺ sensor.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-342**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Optimal Catalyst Condition for Preparing Styrenated Phenol

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¹*Department of Chemical Engineering, Suncheon National University, Korea*

Technical mixture of styrenated phenols including mono-, di-, and tri-styrenated phenol, and TSP has been commonly applied for industrial materials such as rubber or plastic stabilizer, antioxidant, and nonionic surfactant, etc. Among these styrenated phenols, di-styrenated phenol should be most effective as rubber and plastic stabilizers. Although a number of catalysts for the synthesis of styrenated phenols have been explored, researches on the synthesis of styrenated phenol generally have been focused to selective preparation of mono-styrenated phenol MSP, rather than di-styrenated phenol DSP. In this study, we have investigated the hydroarylation reaction of styrene with phenol to find the optimal catalyst, including single catalysts and mixed catalysts, to get high selectivity to DSP under mild reaction conditions.

Conference Date: October 18~20, 2017

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Code: **ORGN.P-343**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dual Chemosensor based on Spiropyran-Isoquinoline Dyad

yongmin ko, Eun Ju Shin*

Department of Chemistry, Suncheon National University, Korea

Spiropyran derivatives have been extensively studied as typical photochromic molecules. The colorless non-fluorescent spiropyran form is converted into colored fluorescent merocyanine form upon ultraviolet (UV) irradiation. The neutral spiropyran form cannot act as a chelating ligand for metal cations. The negatively charged phenolic oxygen in the zwitterionic open merocyanine form, which is produced from spiropyran on UV irradiation, efficiently binds with protons and metal ions. We have prepared Spiropyran-Isoquinoline dyad 1 with isoquinoline ring incorporated into spiropyran as a dual chemosensor for both Co^{2+} and In^{3+} cations. Dyad 1 is expected to be very efficient chelating ligand because both the negatively charged phenolic oxygen and isoquinoline nitrogen may bind cooperatively with protons and metal cations. A new Spiropyran-Isoquinoline dyad 2 with different linkage between spiropyran and isoquinoline has been synthesized to contain more nitrogen in the linkage. In this study, spectroscopic properties of dyads 1 and 2 have been investigated and their metal cation-sensing ability has been comparatively examined.

Conference Date: October 18~20, 2017

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Mixed Catalysts to Obtain the High Selectivity of Distyrenated Phenol

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Department of Chemistry, Suncheon National University, Korea

¹*Department of Chemical Engineering, Suncheon National University, Korea*

Addition reaction of styrene to phenol in the presence of catalyst gave the mixture of styrenated phenols, which are composed of o-mono-styrenated phenols (o-MSP) and p-mono-styrenated phenols (p-MSP), o,o-di-styrenated phenols (o,o-DSP) and o,p-di-styrenated phenols (o,p-DSP), and o,o,p-tri-styrenated phenol (TSP). Technical mixture of these styrenated phenols is important industrial materials and has been widely used as rubber or plastic stabilizers, antioxidant, and nonionic surfactant, etc. These reactions are usually assisted by either protic acid or Lewis acid. However, these methods have several limitations like the use of stoichiometric amount of Lewis acids, drastic reaction conditions (i.e. high temperature, longer reaction time etc.), lower selectivity, over alkylation products and large amount of salt and waste formation. Thus, identification of an efficient mixed catalytic system for hydroarylation of alkenes remains an intriguing challenge. In this work, hydroarylation of styrene with phenol was studied to obtain the high selectivity of distyrenated phenol, using various mixed catalyst in mild condition.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Spectroscopic Properties of Rhodamine-Coumarin Dyad

HyeonSuk JO, Eun Ju Shin *

Department of Chemistry, Suncheon National University, Korea

Rhodamine dye has excellent photophysical performances, such as long wavelength absorption and fluorescence emission located in the visible region, making it a nice platform for fluorescent molecular sensor design. Spirolactam ring-closed form of rhodamine derivatives are nonfluorescent and colorless, whereas ring-opened form of rhodamine derivatives gives rise to strong fluorescence emission and a pink color. Due to the metal cation-induced color and fluorescence changes, rhodamine-based chemosensors have been extensively studied. Coumarins are water soluble, UV-excitabile, and blue fluorescent dyes (emission range ~410 to 470 nm). We report here the preparation and spectroscopic properties of rhodamine-coumarin dyad as a candidate of chemosensor for a specific metal cation.

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Venue: Kimdaejung Convention Center, Gwangju

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Preparation and Spectroscopic Properties of Rhodamine-Quinoline Dyad

DaeWon Jung, Eun Ju Shin*

Department of Chemistry, Suncheon National University, Korea

Rhodamine dyes have always received high-level attention because of their excellent photostability, high absorption coefficient, strong fluorescence in the visible region, and water-solubility. In recent years, selective optical receptors for the detection of environmentally and biologically important metal cations have received extensive attention for designing and development of colorimetric and fluorimetric chemosensors. Rhodamine derivatives are widely used as chemosensor for various metal cations. Ring-closed spirolactam form of rhodamine is colorless and non-fluorescent, whereas ring-opened form of rhodamine formed by the addition of metal cations is pink-colored and strongly fluorescent. We report here a rhodamine-based colorimetric sensing probe for the selective detection of metal cation. Rhodamine-Quinoline dyad has been prepared and characterized by IR, ¹H NMR, and ¹³C NMR spectra. Its absorption and fluorescence spectroscopic properties have been investigated.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

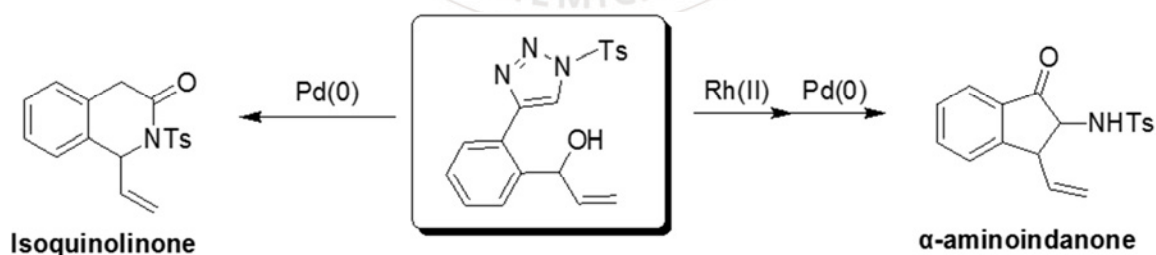
Divergent Transformations of Allyl Alcohol tethered N-Sulfonyl-1,2,3-Triazoles into α -Aminoindanone and Isoquinolinone Derivatives

Dajung Jung, Kyu Ree Lee, Sang-gi Lee^{1,*}

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

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

Divergent catalytic reaction provide quick access to structurally different compounds from a common precursor through controlled reaction pathways. N-sulfonyl-1,2,3-triazoles are the facile precursors inducing various derivations via rhodium(II)-carbene intermediates. Recently, there has been rapid development in intramolecular pathways of the typical carbene or thermal reaction introducing bromide, alkoxy, allylic ether groups mediated N-sulfonyl-1,2,3-triazoles. The new transformations of allyl alcohol tethered N-sulfonyl-1,2,3-triazoles have been developed, affording divergent synthesis of isoquinolinone and 1-indanone derivatives according to two different catalytic reaction conditions (Scheme 1).



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of N-heterocyclic carbene(NHC) catalysts for bisalkoxycarbonylation of α -olefins

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¹*Division of Energy System, Ajou University, Korea*

²*Department of Chemistry, Ajou University, Korea*

The carbonylation reaction of olefins is important to convert low value added olefins and CO into high value carbonyl compounds. Among them, we focused on bisalkoxycarbonylation, which produces succinic diesters. The succinic diester, a compound produced by the bisalkoxycarbonylation reaction of olefin, can be used not only in the chemical field but also in the pharmaceutical field. Generally, bisalkoxycarbonylation proceeds based on Pd catalyst. In this case, the ligand is mainly phosphine. However, since the phosphine ligands are air sensitive, they have a disadvantage in that the reaction conditions are difficult because of the stability. In contrast, NHC (N-heterocyclic carbene) ligands affect the electron donation to the vacant p-orbital of carbene adjacent to the lone pair of hetero atoms. This plays a major role in the stability of the NHC ligand. Thus, we synthesized a catalyst using an NHC ligand that is more stable than the phosphine ligand and has σ -donating ability corresponding to the phosphine ligand. This catalyst was used for efficient synthesis of succinic diester.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-349**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Terpolymerization of CO, Ethylene and Propylene using Pd-complexes; The Size Effect of Heterogeneous Acid Additives

Yeon Joo Cheong, yuna Lim, Shin Young Kang¹, Seung Uk Son^{1,*}, Hye-Young Jang^{2,*}

Division of Energy System, Ajou University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

²*Department of Chemistry, Ajou University, Korea*

Recently, the study of global warming solution is done actively. Especially, chemical conversion using C1 gas such as CO, CO₂, CH₄ can be the solutions of global warming. Synthesis of polyketones is one of them. It has been synthesized from CO gas as C1 feedstock in the presence of a palladium catalyst. Thermoplastic polyketones attract great attention to the polymer industry due to its various physical properties. Nevertheless, polyketones has two problems. One is a reactor fouling and the other is that it contains high melting temperature(T_m). In the presentation, we present a new polyketone catalyst composition involving palladium catalyst and MON-SO₃H for resolve the reactor fouling problem. And by performing terpolymerization which use propylene additionally, we decrease the T_m to 230°C. We used several size of MON-SO₃H. Because of its different size, it can control catalytic activity and solve reactor fouling problem. Detail reaction conditions and the effect of different size of MON-SO₃H are discussed.

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Code: **ORGN.P-350**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

α -Sulfonylation of Carbonyl Compounds *via* Organic Catalytic Process

Hyeong-Wan Noh, Hye-Young Jang^{1,*}

Department of Energy System, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Carbon-sulfur bonds are important role as valuable and attractive synthetic intermediates. Among them, α -sulfonylated compounds are used as building blocks in pharmaceutical, industrial processes. And important intermediates for the synthesis of heterocycles, β -ketosulfones, α,β -unsaturated carbonyl compounds and others. Previously, our research group reported the catalytic synthesis of sulfenamides using thiol and confirmed that sulfenamide can be used as a sulfonylating agent. In this conferences, I would like to present detailed conditions for the formation of α -sulfonylated carbonyl compounds using sulfenamides.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

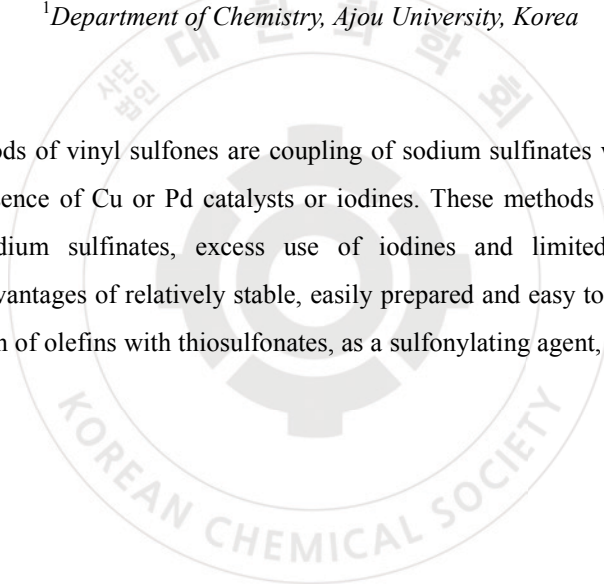
Cu-catalyzed sulfonylation of olefins with thiosulfonates

Soobin Son, Hye-Young Jang^{1,*}

Department of Energy System, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Known synthetic methods of vinyl sulfones are coupling of sodium sulfinates with aryl halides, alkenes and alkynes in the presence of Cu or Pd catalysts or iodines. These methods have limitations of using relatively unstable sodium sulfinates, excess use of iodines and limited commercial resources. Thiosulfonates have advantages of relatively stable, easily prepared and easy to handle. In this study, we present the sulfonylation of olefins with thiosulfonates, as a sulfonylating agent, in the presence of copper catalyst.



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Area: Organic Chemistry

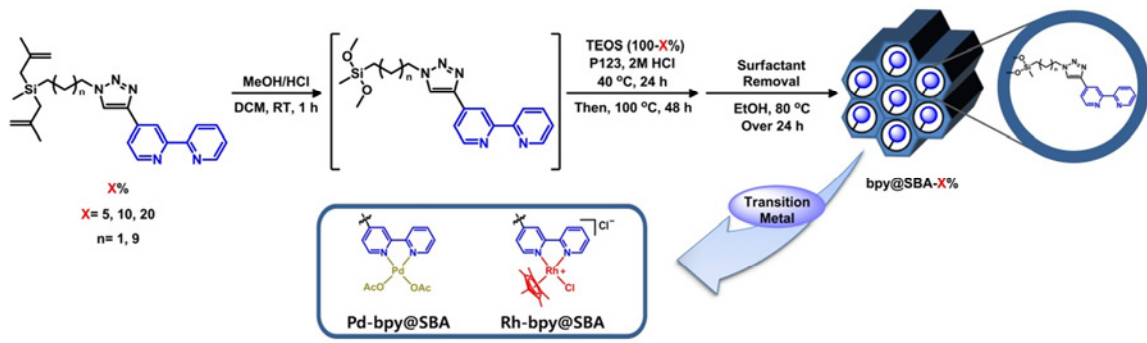
Type: Poster Presentation, Time: FRI 13:00~14:30

Co-condensation synthesis of functionalized mesoporous SBA-15 using methoxysilane derivatives derived from methallylsilane and its application to Catalytic Reaction

JAE SOON KIM, Ye Ri Han, Chul-Ho Jun^{*}

Department of Chemistry, Yonsei University, Korea

In this study, we want to report preparation of metal-coordinated mesoporous silica, SBA-15, and its recyclability as catalyst. Bipyridyl group-introduced dimethallylsilanes are readily prepared by [2+3] Click reaction, which can be readily purified by column chromatography. These methallylsilanes are converted to methoxysilane in an acidic condition using methanol. In preparation of functionalized SBA-15 by co-condensation method, we expected that methoxysilanes might work more effective than methallylsilanes in aqueous reaction condition, since methoxysilanes are easily dissolved in the reaction media due to their hydrophilic character compared to methallylsilanes. That is the reason for converting methallylsilane derivatives to methoxysilane derivatives for introducing more functional groups in SBA-15. By coordinating transition metals (Palladium, Rhodium) to 2,2'-bipyridyl group of SBA 15, well-defined heterogeneous catalysts are prepared, and confirmed by TEM and ICP-MS. These materials are applied to C-H borylation and hydrogenation. For example, Pd-bpy@SBA is used for obtaining alkyl aryl ketone through C-H activation and borylation. In addition, Rh-bpy@SBA is also used for selective hydrogenation by transforming methyl 4-formylbenzoate to methyl 4-(hydroxymethyl)benzoate. These heterogeneous catalysts can be recycled without loss of reactivity.



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Type: Poster Presentation, Time: FRI 13:00~14:30

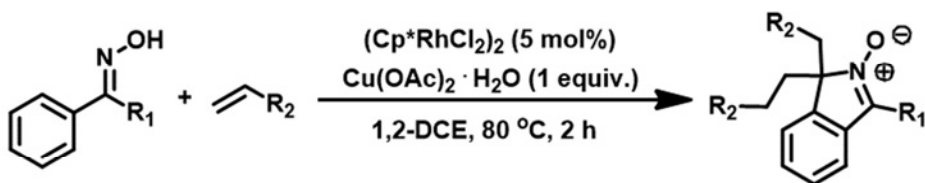
Rhodium(III)-Catalyzed C–H Activation Forming Nitrones Containing a Quaternary Carbon Center from Oximes

Woojin Park, hyejeong lee¹, Chul-Ho Jun^{*}

Department of Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Dong-A University, Korea*

Nitrone derivatives are known to be useful precursor for constructing promising active biological compounds and radical spin-trapping agent. In this research, we describe rhodium(III)-catalyzed one-pot synthesis of nitrone derivatives which have quaternary carbon center from oximes and electron-withdrawing group-substituted alkenes in presence of $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$. The reaction takes place at 80 °C for 2 hours through rhodium(III)-catalyzed chelation assisted C-H bond activation to give corresponding nitrone compounds in high yield. This reaction method is novel in terms of preparation of nitrone compounds containing quaternary carbon center, and its advantageous feature includes atom-economy. The proposed reaction mechanism will be discussed.



R₁ = alkyl, aryl
R₂ = Electron-withdrawing group

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Area: Organic Chemistry

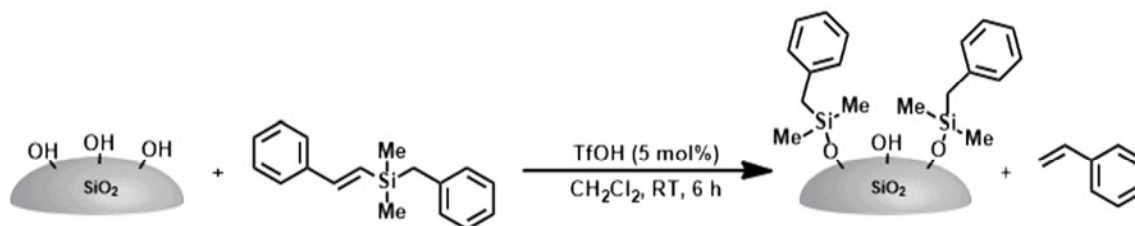
Type: Poster Presentation, Time: FRI 13:00~14:30

Development of efficient immobilization of organic molecules onto silica surface using readily preparable styrylsilane

Soobin Kim, Chang-Hee Lee, Chul-Ho Jun *

Department of Chemistry, Yonsei University, Korea

Immobilization of organic molecules onto solid surface is important in the field of preparation of hybrid materials. In order to immobilize functional organic molecules onto solid surface, the coupling reagent is very important. The most commonly used coupling reagent is alkoxy silanes, but it is unstable and difficult to be purified. To overcome this problem, allylsilane and methallylsilane have been proposed. However, long reaction time and reflux condition is required for activation of allylsilane. To evade these defects, methallylsilane was introduced for immobilization using acid catalyst. Since methallyl group in methallylsilanes is introduced by allyl Grignard reagent, it is difficult to prepare methallylsilyl group in large quantity. In this study, we tried to overcome these defects occurring in conventional immobilization method. One of protocols to solve these is to use styrylsilane. Styrylsilane can be prepared by hydrosilylation of phenylacetylene with silane under transition metal catalyst such as Rh or Pt complexes. Using this protocol, styrylsilane can be prepared in large quantities. In addition, since the styrylsilanes are stable without acid catalyst, it is readily purified by column chromatography. Styrylsilane derivatives prepared by this method can be readily immobilized onto silica surface using a TfOH catalyst at room temperature and shows high immobilization efficiency.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Thermodynamically controlled highly stereoselective tandem Diels-Alder reaction to construct the core of aflavinine

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College of Pharmacy, Korea University Sejong Campus, Korea

A number of indole diterpenoids have been isolated from fungal sclerotia and have attracted attention from the synthetic organic chemists. Due to its unique framework and stereochemistry, we were intrigued by aflavinine among the alkaloids and set out the total synthesis of Aflavinine. Our retrosynthetic strategy features a tandem intramolecular Diels-Alder reaction as a key step. We expect the tandem intramolecular Diels-Alder reaction would provide a rapid access to the synthesis of subtarget of Aflavinine in a highly stereoselective manner and also develop as an useful tool for construction of many complex molecules. We succeeded in synthesizing the core structure of aflavinine which was verified through X-ray crystallography.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Decarboxylative Oxytrichlorination of Arylpropionic Acids with Trichloroisocyanuric Acid

Aravindan Jayaraman, Kye Chun Nam^{*}, Sunwoo Lee^{*}

Department of Chemistry, Chonnam National University, Korea

2,2,2-Trichloroacetophenone derivatives were synthesized from arylpropionic acids and trichloroisocyanuric acid (TCCA). The reaction was conducted in the presence of H₂O at room temperature, and afforded the desired products in good yields. The reaction showed good functional group tolerance towards halides, cyano, nitro, ketone, ester and aldehyde groups. In addition, 2,2,2-trichloroacetophenone derivatives were readily transformed into esters, amides, and hydrazides. Based on experiments with H₂O¹⁸, we proposed two different reaction pathways for aryl- and alkyl-substituted propionic acids.

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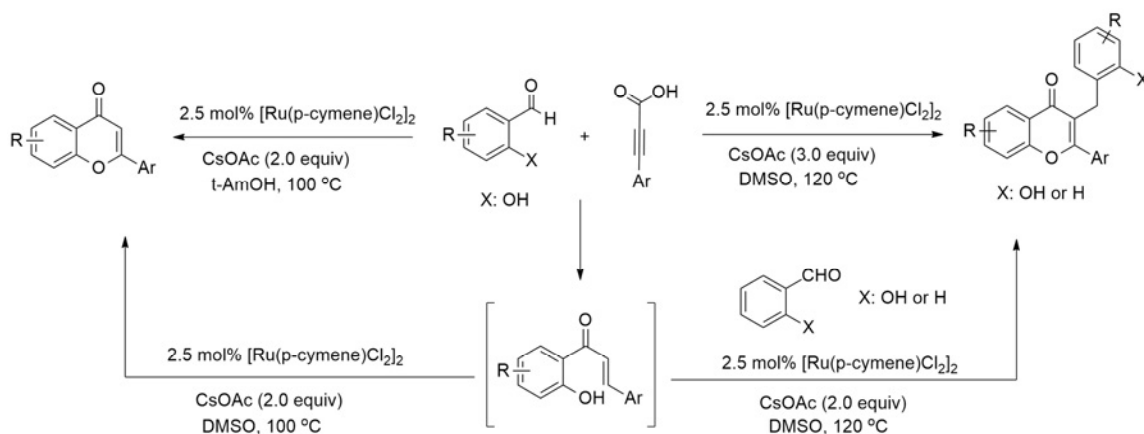
Type: Poster Presentation, Time: FRI 13:00~14:30

An Unprecedented Synthesis of Homoisflavonoids via Ruthenium Catalyzed Decarboxylative Hydroacylation of Aryl Alkyne Carboxylic Acids and Salicylaldehyde

Charles Edwin Raja Gabriel, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Flavonoids are heterocyclic compounds having oxygen atoms and consist of chromone as a core structure. As their analogues, homoisflavonoids are a type of flavones with benzyl moieties at C-3 position. Homoisflavonoids have been found in natural product and known to play important roles such as symbiotic nitrogen fixation, plant pigmentation and UV filtration. In addition, their biological properties such as anti-inflammatory, antioxidant, anticancer, antiangiogenic, antidiabetic, antiallergic, antiviral and antimicrobial activities have been reported. Nevertheless, much efforts for the development of efficient synthetic routes has not been conducted. However, the known methods have drawbacks with respect to requisite multistep synthetic route. When phenylpropionic acid and salicylaldehyde were reacted in the presence of ruthenium catalyst which unexpectedly formed homoisflavonoid. As part of our ongoing studies for the expansion of decarboxylative coupling reactions, more efficient methodology, new synthetic route is being developed for the synthesis of homoisflavonoid.



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Area: Organic Chemistry

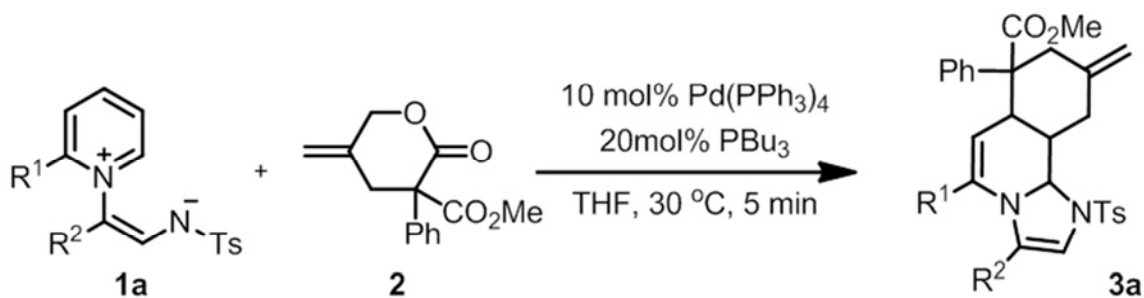
Type: Poster Presentation, Time: FRI 13:00~14:30

Pd-catalyzed site-switchable [4+2] cycloaddition of pyridinium zwitterion with γ -methylidene- δ -valerolactone

Ju Young Lee, Eun Jeong Yoo *

Department of Chemistry, Kangwon National University, Korea

Cycloadditions constitute one of the most important classes of organic reactions giving access to complex organic skeleton in a single step operation which play a key role in the synthesis of natural products, pharmaceutical agents or synthetic materials. Recently, our group discovered that the pyridinium zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners. Interestingly, the cycloaddition of pyridinium zwitterion and nucleophilic palladium-TMM species efficiently provided the site-switchable [3+2] cycloadducts where new bonds were formed on C3- and C4-positions of pyridinium zwitterion instead of [5+3] cycloadducts. In presence of Pd-catalysts γ -methylidene- δ -valerolactone generates nucleophilic 1,4-dipolar species through decarboxylation. In this symposium, we will discuss Pd-catalyzed site-switchable reaction of pyridinium zwitterion with γ -methylidene- δ -valerolactone to provide [4+2] cycloadducts efficiently. In the presence of electron-donating Phosphine ligand PBU₃, the product formation increases effectively perhaps due to increase of nucleophilicity of in situ generated 1,4-dipole.



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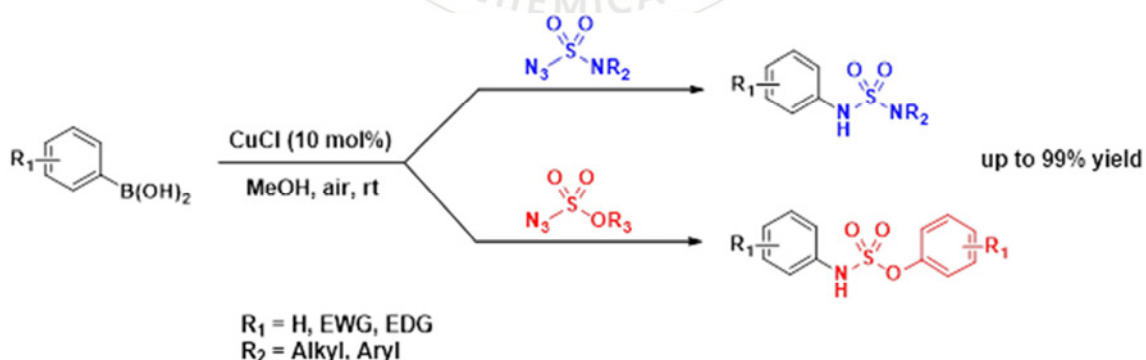
Copper-Catalyzed Synthesis of *N*-Aryl Sulfamides and Phenyl Sulfamates using Organo Azides and Boronic Acids

Suk-Young Won^{*}, Wonsuk Kim¹

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

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

N-aryl sulfamide or phenyl sulfamate moiety is a pervasive entity found in many therapeutic compounds for medicinal chemistry. To the best of our knowledge, the synthesis of *N*-aryl sulfamide is only reported using a sulfamide and an aryl halide in the presence of palladium catalyst until now. Therefore, herein, we report a new copper-catalyzed synthetic method for the preparation of *N*-aryl sulfamides and phenyl sulfamates employing organic azides and boronic acids. Importantly, in the presence of 10 mol% of CuCl, a variety of arylboronic acids were transformed into *N*-aryl sulfamides or phenyl sulfamates at room temperature in 1 h with good to excellent yields in an open flask.



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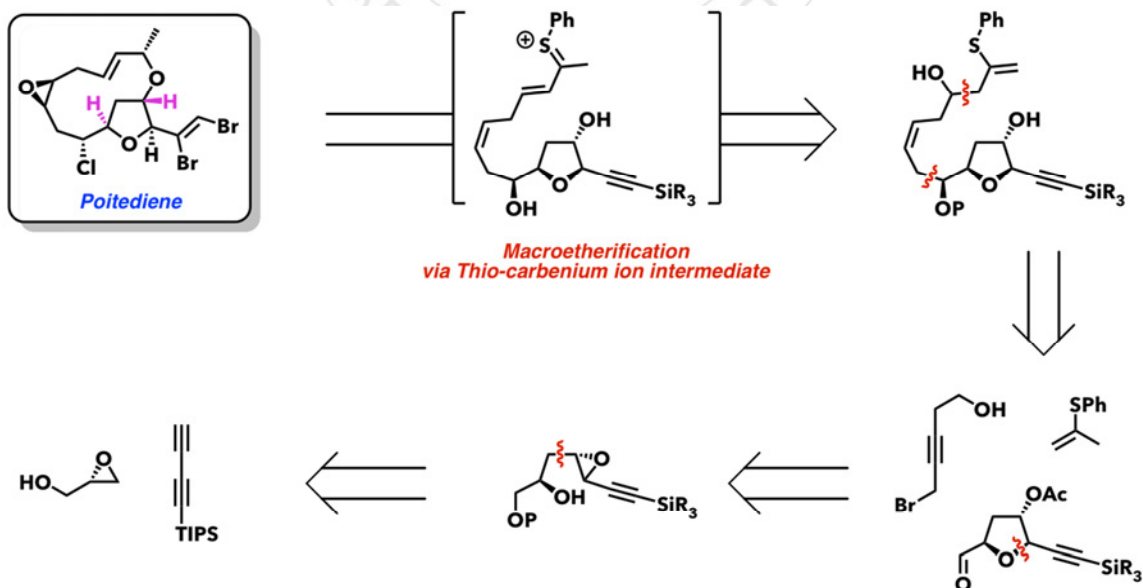
Studies toward the Total Synthesis of Poitediene

Seonwoo Kim, Sinae Kim¹, Robert Matunas¹, Chulbom Lee^{*}

Department of Chemistry, Seoul National University, Korea

¹*Department of Chemistry, Princeton University, United States*

We present here a novel approach to the enantioselective total synthesis of poitediene, a metabolite of red algae possessing a unique “in-out” bridged cyclic structure. We envision that the highly strained 12-membered macrocyclic ether is constructed by etherification using a hetero atom-stabilized carbocation intermediate. The oxolane core was built from epoxy alcohol by zinc-catalyzed etherification, which took place via stereospecific cycloisomerization. Described in this poster are the details of our synthetic route that provides efficient access to the highly functionalized 2,12-dioxabicyclo[9.2.1]tetradecane system.



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Code: ORGN.P-361

Area: Organic Chemistry

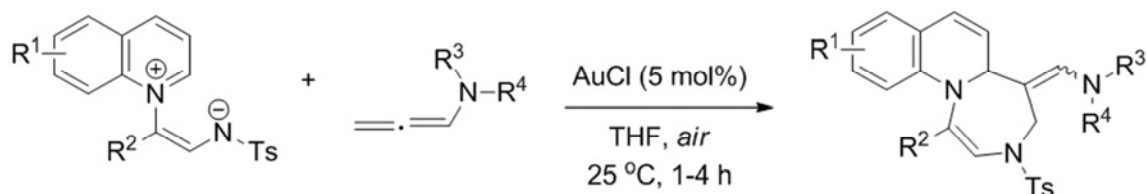
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of fused 1,4-Diazepenes through Au(I)-catalyzed [5+2] Cycloadditions of Allenamides with Quinolinium 1,5-dipoles

Nirupam De, Eun Jeong Yoo^{*}

Department of Chemistry, Kangwon National University, Korea

Polycyclic heterocycles are the core skeletons in a significant number of natural products and biologically active compounds. Especially, fused 1,4-diazepine compounds such as Alprazolam, Bretazenil, and Flumazenil are of particular interest in the field of pharmaceutical chemistry. Metal-catalyzed dipolar cycloadditions are one of the most powerful and widely used synthetic methods for the construction of heterocycles. Although plenty of examples are found where dipolar cycloadditions are applied to synthesize five and six membered heterocycles, there are only few reports of higher order dipolar cycloadditions. Recently, our group discovered that a pyridinium zwitterion with unusual type charge distribution could serve as 1,5-dipole for the synthesis of seven and eight-membered heterocycles via 1,5-dipolar cycloadditions. Herein, we explore a new type of intermolecular gold(I)-catalyzed [5+2] cycloaddition between quinoline-based 1,5-dipoles with allenes. The developed 1,5-dipolar cycloaddition of quinolinium zwitterions occurs at room temperature leading to the formation of fused 1,4-diazepene derivatives with high efficiency.



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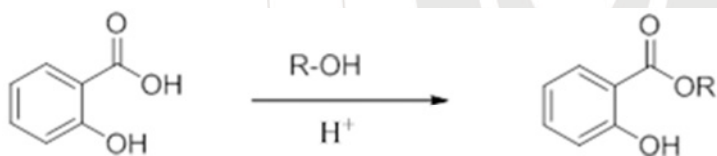
Type: Poster Presentation, Time: FRI 13:00~14:30

The Convenient Preparation of Salicylate Derivatives; Applications of Aroma Chemicals

Ji eun kim, Chujin Ahn*

Department of Chemistry, Changwon National University, Korea

The salicylate derivatives have been known as aroma chemicals and medicine. The known and new salicylate derivatives were prepared conveniently in our lab, and we investigated fragrance of the prepared salicylate derivatives.



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Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of 1,3,5-triazacyclohexane derivatives using amino acids and their use in delivery of nucleic acid therapeutics materials

Soo Kyung Cho, Eunbi Kim, Dai Il Jung^{*}, JUNGTAI HAHN¹

Department of Chemistry, Dong-A University, Korea

¹*Department of Beauty Care, UI University, Korea*

RNA interference (RNAi), a disease gene disruption strategy with enormous potential, can be achieved by delivering small interfering RNA (siRNA) to target tissues effectively and safely. A major consideration in RNAi is the choice of the delivery vehicle. Dendrimers, which are useful candidates for the delivery vehicle, have properties such as highly defined structure, multivalency, and molecular uniformity and are biologically active under the influence of peripheral groups and generation numbers. In addition, a number of studies have suggested that the flexibility of the core play an important role in the biological activity. Although dendrimers causes toxicity problems due to large molecular weight and large surface area, it also promise many advantageous properties such ase extremely low polydispersity and molecular homogeneity. In this study, stimuli-responsive 1,3,5-triazacyclohexane are synthesized from amino acids such as cysteine, glycine and serine with biodegradable branches. Incorporating biodegradable linker in the branch is expected to decrease the cytotoxicity as well as possible side effects.

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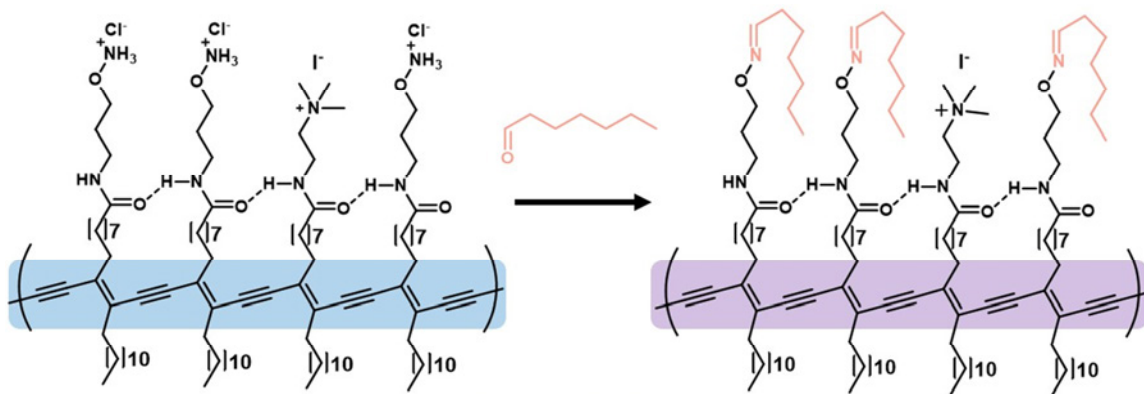
Type: Poster Presentation, Time: FRI 13:00~14:30

A colorimetric sensor for heptanal as a lung cancer biomarker using hydroxylamine-functionalized polydiacetylene

Jinyoung Oh, Seungyoon Kang, Cheol Gyu Lee, Min Su Han^{*}

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

It is essential to develop a detection method for heptanal, since it can be used as a biomarker of lung cancer. In this study, a colorimetric sensor for heptanal was developed, using hydroxylamine-functionalized polydiacetylene (PDA). The hydroxylamine group of the PDA liposome reacts with the aldehyde group of heptanal and facilitates the penetration of the alkyl chain of heptanal into the PDA liposome. From the interactions, the consequent perturbations in the backbone result in blue-to-red color transition, allowing colorimetric detection by the naked eye. The chemosensor had an estimated detection limit of 4.8 μM , with selectivity for heptanal over formaldehyde and acetaldehyde. The efficacy of the heptanal detection method developed in this study was applicable with tap water and serum samples.



Control Heptanal Hexanal Valeraldehyde Butyraldehyde Propionaldehyde Acetaldehyde Formaldehyde Benzaldehyde Glutaraldehyde



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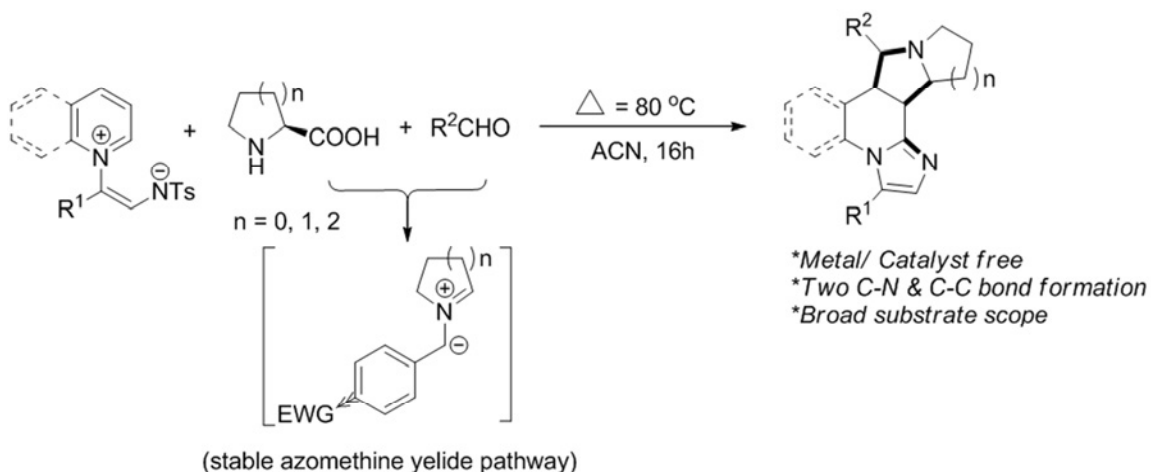
Type: Poster Presentation, Time: FRI 13:00~14:30

Metal Free Decarboxylative [3+2] Cycloaddition: An Easy Access to Polycyclic Fused Pyrrolizidines

Srinivas Samala, Eun Jeong Yoo *

Department of Chemistry, Kangwon National University, India

Metal free decarboxylative cyclization of amino acids with aldehydes and alkenes leads to polyheterocyclic compounds always has significant role in the synthetic organic chemistry. With this concept, we have successfully developed a methodology for the synthesis of polycyclic fused pyrrolizidines derivatives via metal free multicomponent decarboxylative [3+2] cycloaddition pathway. The resulted compounds seem to have medicinal significance, which includes three important heterocycles: quinoline/ pyridine, imidazole and pyrrolizidines within the one molecule. The interesting fact is note that the regioselectivity of the final compounds depends on the substitution which is present on aromatic aldehyde. If the substitution on benzaldehydes is electron withdrawing group (4-nitro), the resulted final compounds may proceeds through stable azomethine yelide. The broad functional group tolerance clearly indicated that the wide range applicability of present methodology. The synthetic utility has been carried out of resulted final compounds via oxidation by Pd/C catalyst.



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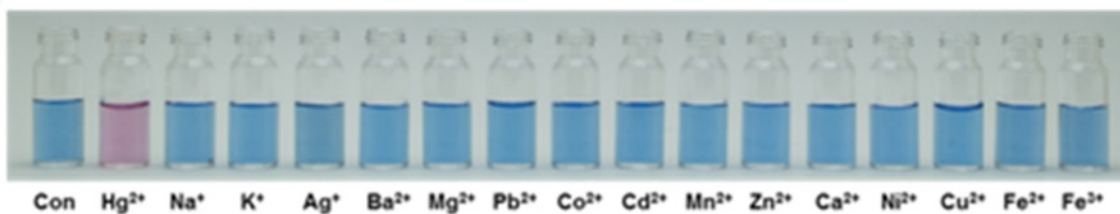
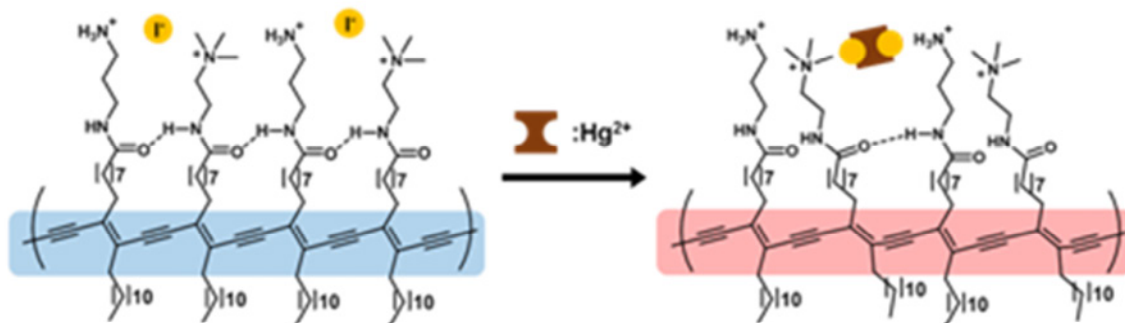
Type: Poster Presentation, Time: FRI 13:00~14:30

A colorimetric and fluorescent chemosensor for detection of Hg^{2+} using counterion exchange of cationic polydiacetylene

Cheol Gyu Lee, Seungyoon Kang, Jinyoung Oh, Min Sik Eom, Min Su Han*

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

In this study, a colorimetric and fluorescent chemosensor for mercury ions (Hg^{2+}) was developed. Cationic polydiacetylene (PDA) vesicles with a quaternary ammonium cation and iodide as a counterion show a blue-to-red color transition; the color change is accompanied by a fluorescence enhancement in selective response to Hg^{2+} ions because of a perturbation of the ene-yne conjugated backbone induced by counterion exchange. It allows for selective detection of Hg^{2+} with the naked eye and the sensor is used to determine Hg^{2+} concentrations in tap water samples.



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Venue: Kimdaejeung Convention Center, Gwangju

Code: ORGN.P-367

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Direct Visualization of Ultrastable Host-guest Interactions in Living Organisms Using Host-guest FRET Pair

Meng Li, ARA LEE¹, Kyung Lock Kim², Gihyun Sung¹, Kyeng Min Park^{3,*}, Kimoon Kim^{4,*}

Center for Self-Assembly and Complexity, Institute for Basic Science, Korea

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⁴*Department of Chemistry, Pohang University of Science and Technology, Korea*

Cucurbit[7]uril (CB[7])-based ultrastable host-guest interactions have shown great potential to replace streptavidin-biotin (SA-BT), by utilizing its ultrastable binding affinity ($K_a \sim 10^{13}$ to 10^{17} M⁻¹) for various bioapplications.^{1, 2} Nevertheless, there has been no direct visualization of the ultrastable interaction between CB[7] and AdA (or FcA) inside living organisms. Here, we directly visualized ultrastable host-guest interactions between CB[7] and AdA in living cells and animal (*Caenorhabditis elegans*) by fluorescence resonance energy transfer (FRET) imaging between cyanine dyes conjugated to host and guest, Cy3-cucurbit[7]uril (Cy3-CB[7]) and Cy5-adamantane (Cy5-AdA). This work demonstrates the potential use of the ultrastable synthetic binding pair as a useful chemical biology tool working inside not only living cells but also animals. References 1. D. W. Lee, K. M. Park, M. Banerjee, S. H. Ha, T. Lee, K. Suh, S. Paul, H. Jung, J. Kim, N. Selvapalam, S. H. Ryu, K. Kim, *Nat. Chem.* 2011, 3, 154-159. 2. D. Shetty, J. K. Khedkar, K. M. Park, K. Kim, *Chem. Soc. Rev.* 2015, 44, 8747-8761.

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Area: Organic Chemistry

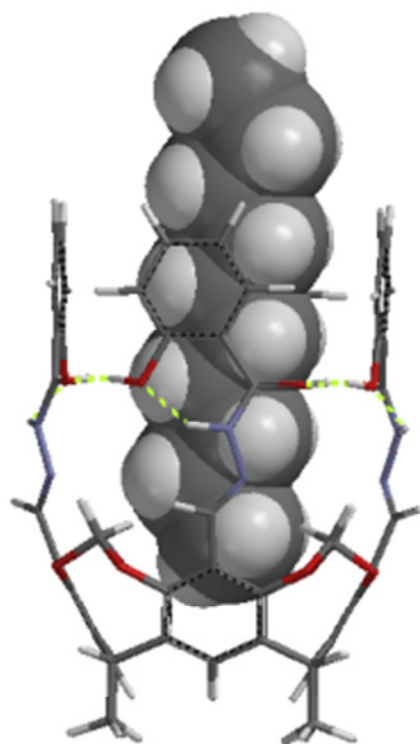
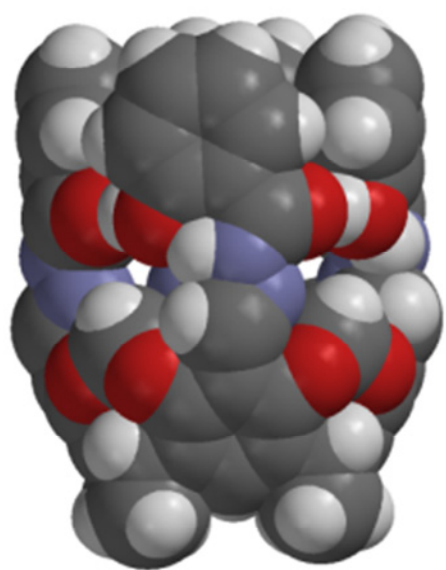
Type: Poster Presentation, Time: FRI 13:00~14:30

Resorcin[4]arene-based hydroxy benzamido-iminocavitand: their complexation and potentials

JUNG SAEGYO, Yang ryeong Kim, Yeon Sil Park, Kyungsoo Paek*

Department of Chemistry, Soongsil University, Korea

Cavitands are synthetic host molecules with open-ended enforced concave cavities large enough to embrace complementary guest compounds. Self-assembling cavitands based on noncovalent interactions have attracted considerable interest due to their potentials as molecular storage, sensor, or catalysts in the field of supramolecular chemistry. The resorcin[4]arene-based 2-hydroxy benzamido-iminocavitand formed stable bowl-shaped conformation in nonpolar solvents by the four intramolecular C=O • • • H • O • • • H-N hydrogen bond sequence in the presence of suitable guests. The synthesis and versatile characteristics of this self-folding cavitand toward neutral guests will be presented.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Cu-Catalyzed Aza-Michael Addition of (Hetero)aryl Amines to Disubstituted Olefins

Seongil Kang, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

Aza-Michael addition of (hetero)aryl amines to disubstituted olefins is one of the simplest and most effective strategies for the synthesis of β -amino carbonyl compounds using readily available alkenes. Among the numerous protocols involving aza-Michael additions, Cu-catalyzed processes are particularly attractive because of the use of environmentally benign and low cost copper salts, and mild reaction conditions. Herein, we developed an efficient NHC-Cu catalytic system for the conjugate addition of a variety of anilines and heterocycles to disubstituted alkenes including sulfonyl group with high efficiency. In addition, we described an efficient phosphine-Cu catalytic protocol for aza-Michael addition of various anthranilates to disubstituted α,β -unsaturated ketones. The synthetic utility of this methodology was demonstrated by the synthesis of the 4-hydroxy-quinoline derivatives, which are useful intermediates in synthetic organic chemistry and valuable building blocks in medicinal chemistry.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Selective discrimination of putrescine and cadaverine based on a Fe³⁺-morpholinoanthracene ensemble

Anup Pandith, HANSOL SEO, Hong-Seok Kim *

Department of Applied Chemistry, School of Applied Chemical Engineering, Kyungpook National University, India

An anthracene-aminomethylpropylmorpholine (1)-Fe³⁺ chelate was designed, synthesized, and characterized. The *in situ*-generated Fe³⁺ ensemble selectively detected putrescine (Put) and cadaverine (Cad) through a *turn-off* response via a decomplexation process in DMSO-H₂O (1:1 v/v) at pH 7.3 (HEPES buffer). The decomplexation aided *turn-off* response by the sequential addition of Put and Cad furnished good association constants [$K_{sv} = 2.30 \times 10^6 \text{ M}^{-1}$, and $9.95 \times 10^5 \text{ M}^{-1}$ in a HEPES-buffered DMSO-H₂O (1:1, v/v%) medium, respectively]. By utilizing complexation/decomplexation processes aided through sequential addition of Fe³⁺ and Put/Cad an INHIBIT photonic logic gate and its fluorogenic tracking was demonstrated in primitive- eukaryotic cell lines.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Total Synthesis of Oryzativols B

Seonju Kim, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

Oryza sativa L., Oryza rice, is a staple food and its roots have been used as medical supplement. Recently, Oryzativols B was isolated from *Oryza sativa* L. and a variety of its biological properties have been studied. However, the synthesis of the natural product was not achieved. Oryzativols B consists of a furan ring as a main scaffold bearing coumaric acids. Herein, we described a synthetic approach to Oryzativols B through esterification of tetraol with *trans-p*-coumaric acid and *cis-p*-coumaric acid derivative. Our synthesis was started from a commercially available 4-hydroxy-3,5-dimethoxycinnamic acid and achieved in 12 steps with 10% overall yield.

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Area: Organic Chemistry

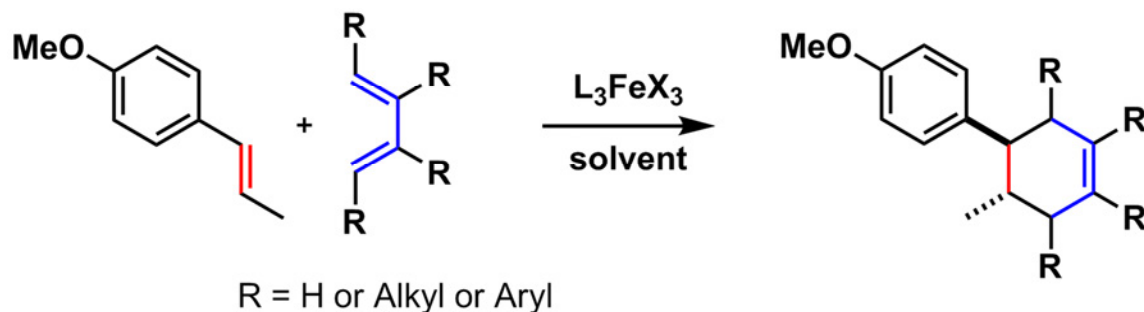
Type: Poster Presentation, Time: FRI 13:00~14:30

Radical Cation Catalyzed Electron-Mismatched Cycloaddition Reaction Using Iron(III)-Polypyridyl Complex

EunYoung Seong, JungHa Shin, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

$\text{Fe}(\text{Phen})_3^{3+}$ complex and its derivatives have sufficient oxidizing potential to act as an one-electron oxidant, thereby promoting efficient radical cation cycloaddition of electron-rich dienophiles. It is known that photocatalysts or organic catalysts conduct electron mismatched Diels-Alder reaction or [2+2] cycloaddition efficiently as an one-electron oxidant via radical cations of electron-rich olefins. Recent study is going along with Ruthenium(II) or Cr(III) complexes as a photocatalyst and came out into open that chain propagation steps dominate product formation in polar radical cycloaddition mechanism compared to initiation step. We performed this reaction using Fe(III) complexes as effective radical generator although these catalysts can't carry out whole catalytic cycle. Going one step forward, we performed varying ligand of Fe(III) complexes that can result in differential reactivity from established organic catalysts. It can be a facile route to replace rare metals with inexpensive iron to make an effective radical cation cycloaddition reaction.



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Area: Organic Chemistry

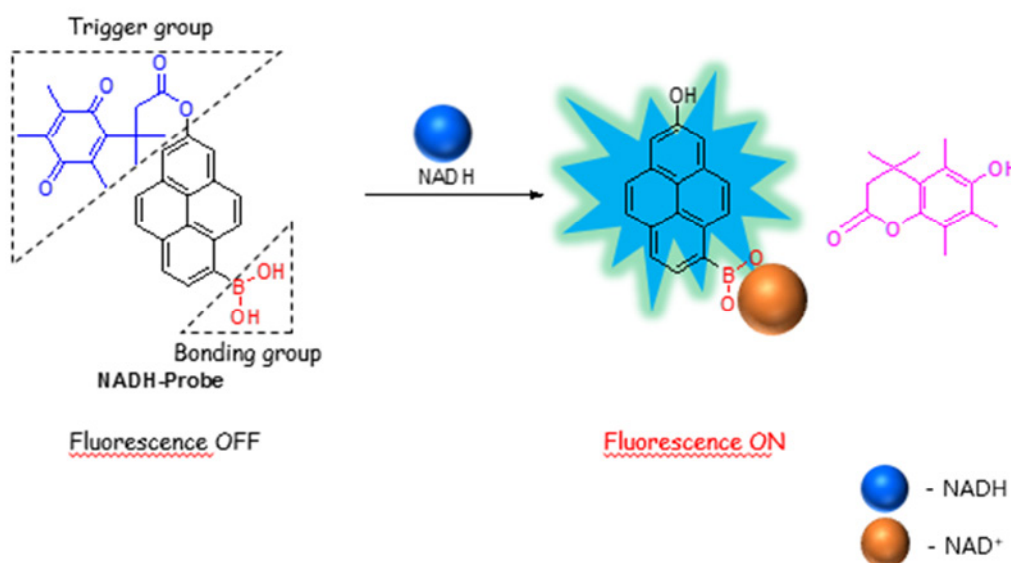
Type: Poster Presentation, Time: FRI 13:00~14:30

A efficient fluorescence probe for sensitive detection of NADH

Sun Woo Lee, tae eun park, Seoung Ho Lee*

Department of Applied Chemistry, Daegu University, Korea

In this study, we report a simple strategy to efficiently detect NADH at the very low concentration levels. A novel fluorescent probe consisting of a boronic acid attached pyrene moiety (fluorophore) and a benzoquinone moiety (quencher) has been developed. The initial probe shows quenched fluorescence via photo-induced electron transfer from pyrene to benzoquinone. NADH sensing studies illustrate that the selective assemblies of boronic acid on the probe with NADH exhibit ratiometric turn-on response in the very low concentration levels, where reduced benzoquinone induces hydrolysis of pyrenyl acetate groups to release pyrenoxy group.



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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-374**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Anionic Conjugated Polyelectrolyte Micelles as Sensitive Mercury(II) Ion Sensor Systems

sujin jung, Euijin Roh, Seoung Ho Lee*

Department of Applied Chemistry, Daegu University, Korea

An amphiphilic fluorophore containing a thioate ionic group and a pyrene moiety on each side of the alkyl chain has been newly designed for a mercury (II) ion sensor. This building blocks give the conjugated polyelectrolyte micelle (CPM) formation along with a very high association for Hg(II), which exhibits a very sensitive and selective turn-on fluorescence response. The π -extended conjugated system in self-assembled CPM allows enhanced optical properties including efficient energy or electron transfer, and high quantum yield.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-375**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

CN⁻ assisted ESIPT Enhancement in Hydroxyphenyl thiazole-vinyldicyano Donor-Acceptor Dyad

HANSOL SEO, Joonhyuk Huh, hoi jo, Hong-Seok Kim^{*}

Department of Applied Chemistry, School of Applied Chemical Engineering, Kyungpook National University, Korea

Probe 1 was prepared from the reaction of 2-(2'-hydroxyphenyl)-4-furnylthiazole and malononitrile. Sensing ability of 1 in various anions were studied and mechanism was postulated based on UV-Vis absorption spectra, fluorescence spectra and NMR studies. Further experimental DFT functional based molecular simulation was studied. Owing to the combined effects of addition of CN to double bond and deprotonation OH proton, 1 could sense CN⁻ with high selectivity and sensitivity. 1 probe detected CN⁻ ion selectively in DMSO with very high binding constant in 1:2 stoichiometry.

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Code: **ORGN.P-376**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Discrimination of Chirality of α -Amino Acids in ZnII Complexes of DPA-Appended Binaphthyl Imine

YINGJI JIN

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

We have synthesized binaphtholic aldehydes dangled with dipicolyl amine moieties, (R)-1, and (R)-2, and studied their reaction with amino acids and ZnII ion. The crystal structure of (R)-1-L-Ser revealed crowded and distorted octahedral coordination sphere around the ZnII ion. ¹H NMR spectra of the complexes obtained from D- and L-amino acids are well discriminated from each other, and thus might be conveniently used as a chiral shift reagent for some amino acids. As for the aldehyde (R)-2, a dimeric Zn(II) complex with an amino acid was generated, which was highly enantiospecific for L-Phe and L-Trp. We developed in this work a new system of the ZnII complex of an amino-acid Schiff base showing chiral discriminations and has a relatively labile binding with a ligand that can lead to easy recovery of the bound amino acid.

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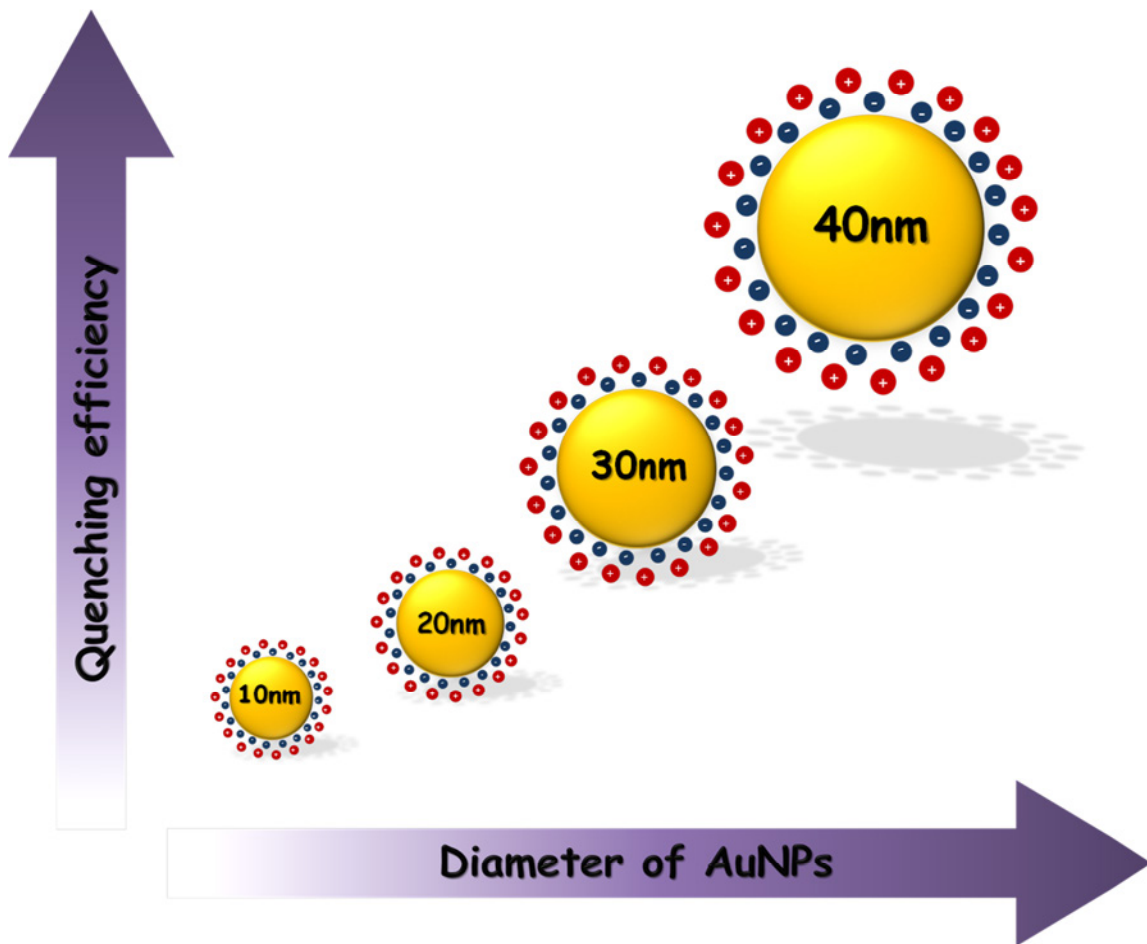
Photoluminescence quenching of water soluble polyelectrolyte on Au nanoparticles

Boyun Kim, Seoung Ho Lee^{*}, Kirk S. Schanze^{1,*}, Gyu Leem^{1,*}

Department of Applied Chemistry, Daegu University, Korea

¹*Department of chemistry, University of Texas at San Antonio, United States*

In this report, we have demonstrated the photoluminescence quenching and energy transfer of water soluble polyelectrolytes, (P-C-3 and P-O-3) with tuning the sizes of Au nanoparticles (e.g. approximately 10, 20, 30, 40 nm) by emission quenching. Simple adjustment of the amount of reducing agents allowed precise tuning of the size of the Au nanoparticles, which were characterized in bulk form by transmission electron microscopy (TEM), dynamic light scattering (DLS). We have described the quenching phenomena by the quenching constant value (K_{SV}). The polymers were efficiently quenched by Au nanoparticles and exhibited 50% emission quenching ($I_0/I = 2$). Stern–Volmer constants for quenching of the polymers showed significant amplification with $K_{SV} > 4.7 \times 10^{12} \text{ M}^{-1}$ using 40 nm Au nanoparticles in comparison to the quenching of the polymer with 10 nm Au nanoparticles ($K_{SV} > 5 \times 10^{10} \text{ M}^{-1}$). The quenching efficiency increases with an increase in the size of the nanoparticles.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Self-assembling fluorescent probes for for an efficient CO₂ detection

JungMoo Lee, sujung Kim, Seoung Ho Lee*

Department of Applied Chemistry, Daegu University, Korea

In this study, we have designed self-assembling fluorescent probes with a fluorophore and an amine group covalently linked via a hydrophobic alkyl chain. These particular probes are self-assembled in a CO₂ environment through noncovalent interactions between carbamic acids, formed by the reaction of amine with CO₂, and unreacted amines. Self-assembled fluorescent probes are more stabilized by hydrophobic interaction of fluorophore attached alkyl chains, giving the self-assembled micelle formation in aqueous solution. Owing to their outstanding optical and structural properties such as π -extended conjugated system at the inner part and hydrophilic groups at the periphery, this micelle formation allows sensitive and rapid monitoring of carbon dioxide with strong fluorescence enhancement at the low concentration levels.

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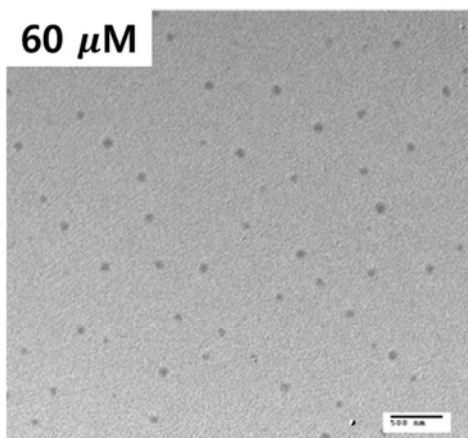
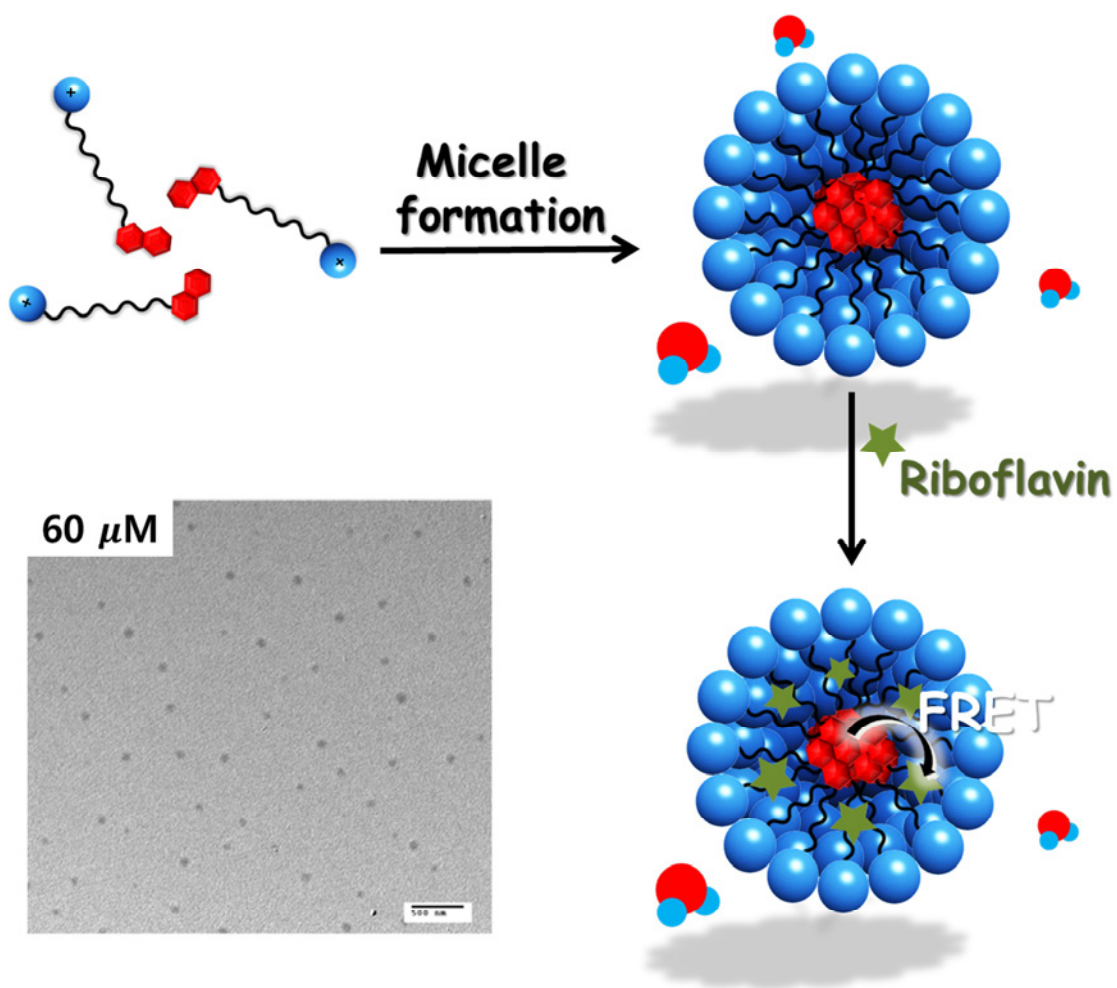
Type: Poster Presentation, Time: FRI 13:00~14:30

A Self-Assembled Conjugated Polyelectrolyte Micelle as an Amplifying Fluorescent Sensory System

Boyun Kim, Yeonjin Jang, Seoung Ho Lee*

Department of Applied Chemistry, Daegu University, Korea

Fluorescence-based assays (FBAs), which are processable in aqueous media, have been explored for use in detection of chemical, biological, radiological, and nuclear agents or elements. However, many FBAs suffer from a low sensitivity that arises from limited sensing transductions for detecting analytes and/or low fluorescence quantum yields induced by reduced excited state energy of fluorophores inherent in aqueous solution. Therefore, the signal amplification for sensing response can provide smart sensory systems for monitoring analytes at very low concentration level. Herein, we demonstrated that a self-assembled conjugated polyelectrolyte micelle (CPM) induces very sensitive signal transduction involving amplified fluorescent changes, which marks a strong difference with the numerous FBAs that have been developed for the sensitive detection. The building block, an amphiphilic coumarin derivative, displays the self-assembled micelle formation in aqueous solution, giving the hydrophobic π -extended conjugated system at the inner part and hydrophilic groups at the periphery. This allows enhanced optical properties, resulting in efficient energy or electron transfer, and high quantum yield. Finally, it is shown that a self-assembled CPM drives highly sensitive detection of RF at low nanomolar concentrations.



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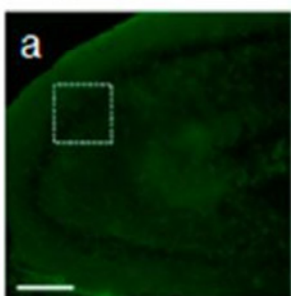
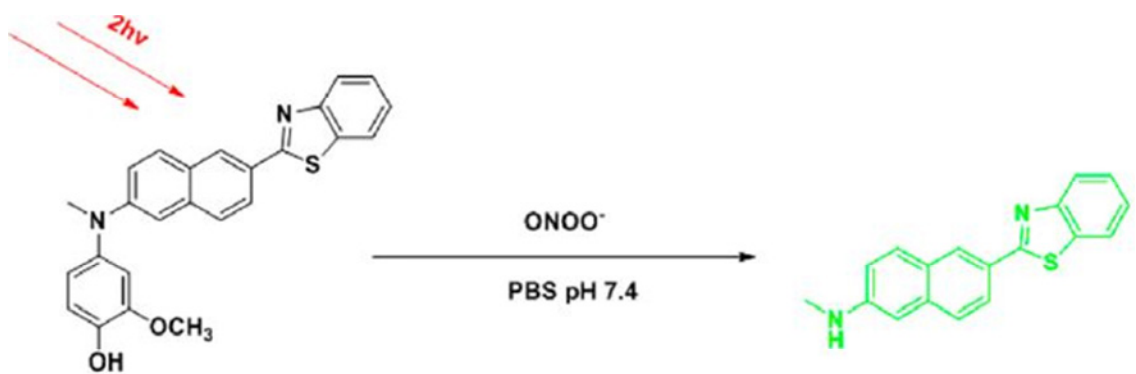
Type: Poster Presentation, Time: FRI 13:00~14:30

Detection of the Endogenous Peroxynitrite in Living Cells and Tissues by a Highly Selective and Sensitive Two-Photon Fluorescent Probe

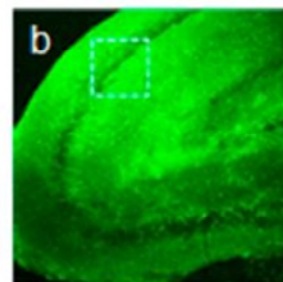
Yerin Jeong, Juyoung Yoon *

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

Peroxynitrite (ONOO⁻), the product of a reaction between the superoxide($\bullet\text{O}_2^-$) and nitric oxide(NO) free radicals, the latter of which is a powerful oxidant that can damage various molecules in cells, including DNA and proteins, has attracted broad interest from the scientific research community. Thus, abnormal levels of ONOO⁻ in cells is implicated in various diseases such as ischemia-reperfusion injury, inflammatory conditions, and neurodegenerative disease. Therefore, detection of ONOO⁻ is useful in the early diagnosis of human disease. Recently, a considerable number of research groups have made an effort to develop ONOO⁻ probes, and many of these probes exhibit good performance in live cells or mice. Herein, a new two-photon fluorescent probe that can detect endogenous ONOO⁻ was designed and synthesized. This new probe exhibits good water solubility, low cytotoxicity, fast response and high selectivity and sensitivity for ONOO⁻ in phosphate-buffered saline solution with a low detection limit. Furthermore, the probe displays good performance not only in RAW 264.7 cells but also in rat hippocampal slices at a depth of approximately 120 μm .



Good water solubility;
High TP cross section;
Low detection limit;
Tissue imaging.



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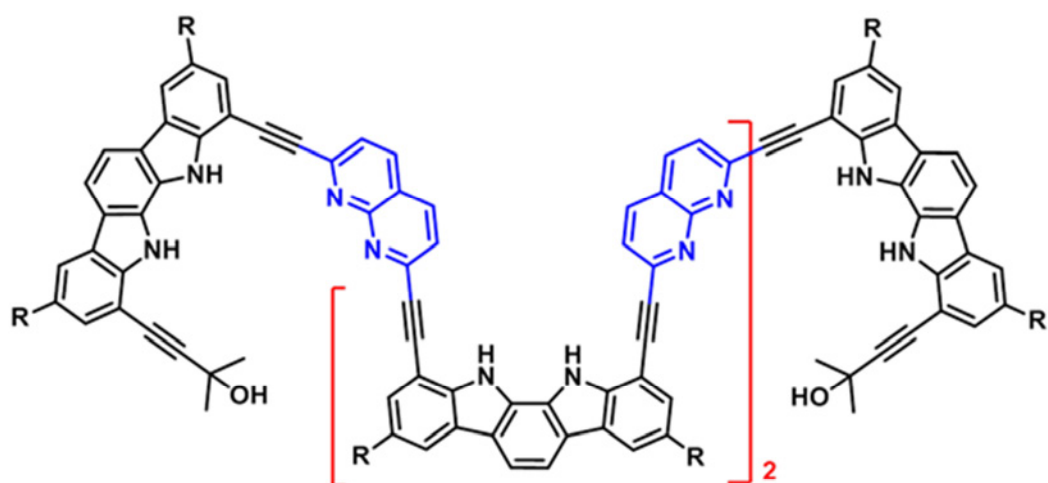
Type: Poster Presentation, Time: FRI 13:00~14:30

An Indolocarbazole-naphthyridine Foldamer Capable of Binding Glucose

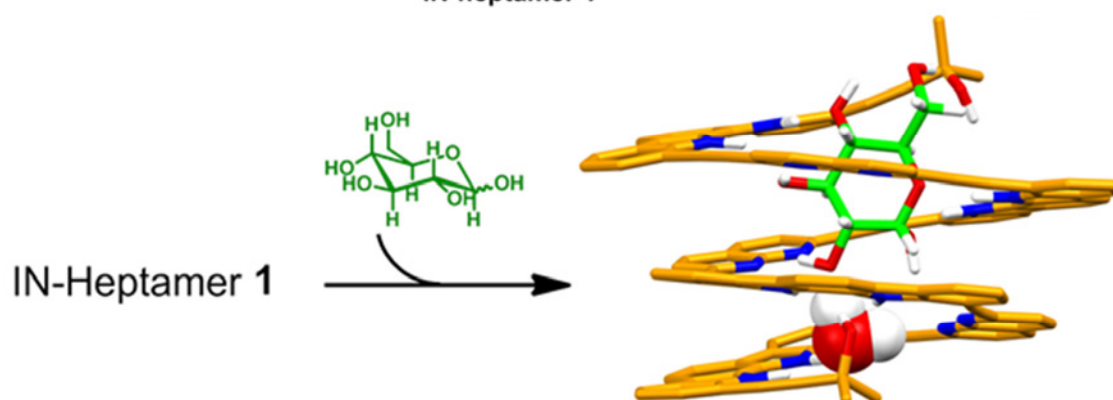
Hae-Geun Jeon, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

An indolocarbazole-naphthyridine foldamer **1** was prepared by alternatively connecting indolocarbazoles and naphthyridines through ethynyl bonds. The foldamer folded into a stable helical conformation with an internal cavity which enwrapped by hydrophilic functional groups; indolic NHs and naphthyridine nitrogens. These helical folding and generation of cavity were clearly revealed by single crystal X-ray structures. The internal cavity could accommodate a glucose molecule, and the binding of the D-glucose induces the biased helical sense to **1**. Therefore, the complex of **1** with D-glucose displays strong circular dichroism (CD). The binding constants of **1** with D-glucose and D-galactose were determined by circular dichroism (CD) titration. Additionally, ¹H NMR signals of D-glucose were dramatically shifted upfield when the D-glucose was bound to **1**. Through computer modeling calculations, we generated a structure of the complex which reflecting the spectral changes of NMR study during the binding event. Details will be described in the poster presentation.



IN-heptamer 1



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Area: Organic Chemistry

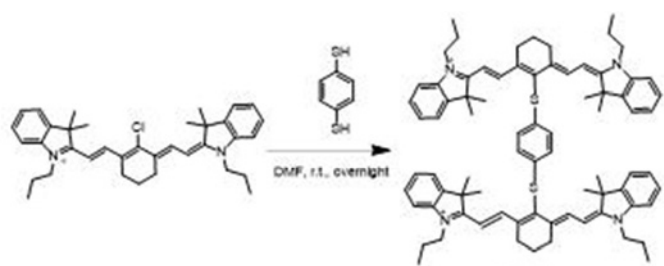
Type: Poster Presentation, Time: FRI 13:00~14:30

The detection of glutathione using Near-infrared fluorescent probes and their application in the fluorescence imaging of living cells and tumors

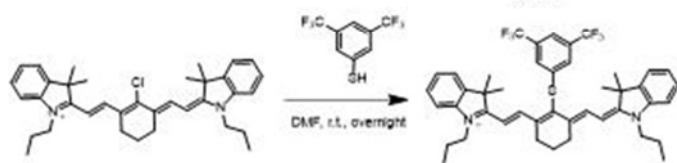
Joohee Hong, Dayoung Lee, Juyoung Yoon*

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

Intracellular glutathione (GSH) is the most abundant intracellular biothiol, present in concentrations from 1 to 15 mmol L⁻¹. GSH is involved in several pathological and biological processes, and plays central roles in the maintenance of intracellular redox homeostasis. Varying GSH concentrations are related to many cellular functions. Therefore, methods to determine the concentrations of GSH in cellular environments and *in vivo* are immediately needed for various biochemical investigations, and the diagnosis of related diseases. Great efforts have been made in developing efficient fluorescent probes for sensing GSH in living cells. Most are based on fluorophores of short or moderate emission wavelengths from 400 to 600 nm, but fluorescent probes with near-infrared (NIR) emissions (650–900 nm) are preferable for *in vivo* imaging. Two NIR fluorescent probes 1 and 2 based on cyanine dye were developed for the detection of GSH. Probe 1 was obtained by integration of two cyanine units into a single molecule, and probe 2 by introduction of a bis(trifluoromethyl)benzenethiol moiety to a cyanine fluorophore. The initial probes are nonfluorescent, and the addition of GSH brought about noticeable enhancement in the NIR fluorescence with high sensitivity. Both probes were applied to imaging varying amounts of GSH in living cells. In addition, the probes can yield *in vivo* fluorescence responses to GSH in tumors.



Probe 1



Probe 2



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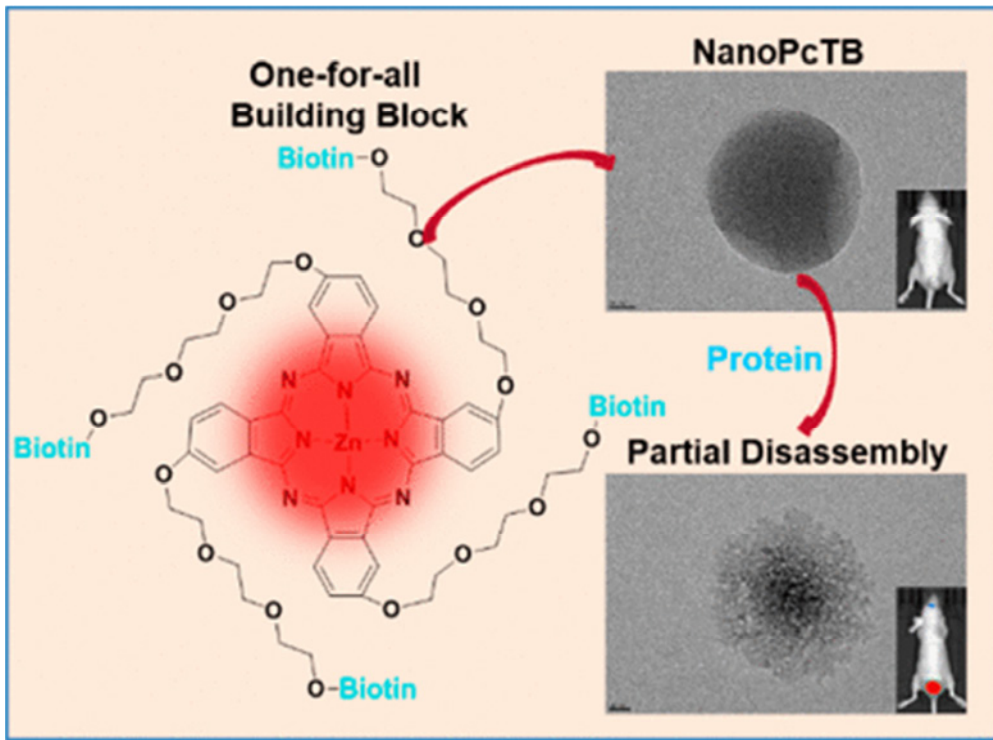
Type: Poster Presentation, Time: FRI 13:00~14:30

Biophotonic Imaging and Therapy by Nanostructured Phthalocyanine Assemblies with Protein-induced Switchable Photoactivities

Sewon Eom, Juyoung Yoon *

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

Switchable phototheranostic nanomaterials gained increasing attention in specific biosensing, high-quality imaging, and targeted therapy in the field of precision nanomedicine. By self-assembling of flexible and versatile phthalocyanine building blocks, we develop a “one-for-all” nanostructured phthalocyanine assemblies (NanoPcTBs). The assemblies show distinctive photothermal and photoacoustic properties. Upon a targeted, protein-induced, partial disassembly mechanism, fluorescence and reactive oxygen species are generated. This enables low-background fluorescence imaging and activatable photodynamic therapy. In vitro evaluations indicate that NanoPcTB has a high selectivity for biotin receptor-positive cancer cells (e.g., A549) compared to biotin receptor-negative cells (e.g., WI38-VA13) and permits a combined photodynamic and photothermal therapeutic effect. For the therapeutic efficacy evaluation, the NanoPcTBs accumulate in A549 tumors of xenograft-bearing mice, and laser irradiation induces the inhibition of tumor growth.



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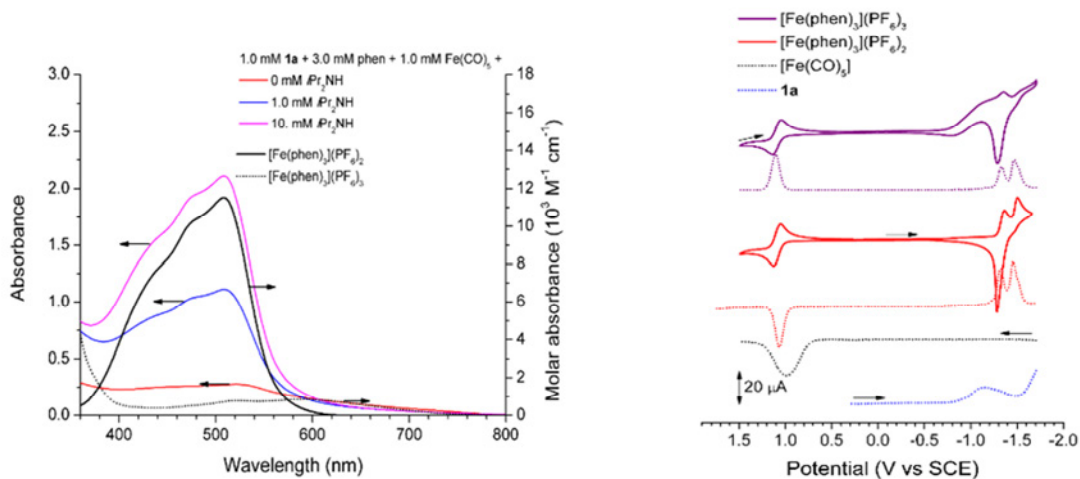
Single electron transfer strategy for reductive cyclization and oxidative cycloaddition reactions using iron polypyridyl complexes

Joon Young Hwang, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Reductive radical cyclization using low-valent iron pentacarbonyl [Fe(CO)₅] to generate radical species from alkyl iodides was achieved. A range of pyrrolidines, tetrahydrofurans, and carbocycles were synthesized via 5-*exo* cyclization reactions of alkyl radical intermediates generated by electron transfer from a system involving Fe(CO)₅, 1,10-phenanthroline, and diisopropylamine. In addition, we have successfully applied to the tandem radical reactions with Michael acceptor. We have found the presence of Fe²⁺(phen)₃ species during the reaction through UV-vis absorption spectroscopy and electrospray ionization mass spectrometry (ESI-MS), which are the distinct evidence that Fe and phenanthroline system acts as electron donor agents. Moreover, we have proved that radical pathway is main route by the radical clock reaction, TEMPO experiment, and electron paramagnetic resonance (EPR) studies to investigate iron(III) complex and phenanthroline radical anion species. Especially, iron(III) polypyridyl complexes can be used as single-electron oxidants with tertiary amines or anilines [$E_{ox} = 0.8-1.0$ V] for formation amine radical cation as a hydrogen atom source. In this regard, we planned oxidative reaction of tertiary amines with iron polypyridyl complexes. 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, we present reductive radical cyclization of iodoalkene and oxidative cycloaddition of tertiary amines with maleimides under mild reaction condition.

Radical generation via SET



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of New Dimeric Fluorescence Probes for Amyloid Aggregates with a Negligible Background Signal *in Vivo* imaging

Seo Won Cho, Kyo Han Ahn*

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

Alzheimer's disease (AD) is a neurodegenerative disorder that progressively destroys memory and induced cognitive decline. The formation of amyloid-beta ($A\beta$) plaques in the specific brain regions is one of the early pathological hallmarks in AD. Several methods to image $A\beta$ plaques have been developed as magnetic resonance imaging (MRI), positron emitting tomography (PET), and single photon emitting computed tomography (SPECT). Among them, Two-photon microscopy (TPM) is an attractive tool for bio-imaging. Many TP fluorescent probes have been developed so far, most of which are based on dipolar dyes; fluorescence increases when it intercalates into $A\beta$ plaque. Although most of probes show a substantial level of background signal, which lowers the signal to noise (S/N) ratio. To overcome this critical issue, we propose a new approach by using the dimeric probes. In our dimeric probe approach, we connected two flat aromatic fluorophores in such a way that the two dyes prefer to exist in folded form, whereas they prefer to exist in unfolded inside $A\beta$ plaques. The folded dimeric probes are in a state of non-fluorescent due to the self-quenching. However, the probes intercalate into β -sheet in $A\beta$ plaques and its binding affinity attenuates the folded formation to be stretched out. The fluorescence is recovered, thus, dimeric probe enabled *in vivo* imaging of $A\beta$ plaques in disease-model mouse, with negligible background signal. These results demonstrate that dimeric probe will be useful in biomedical application including early diagnosis and treatments of AD with less background signal.

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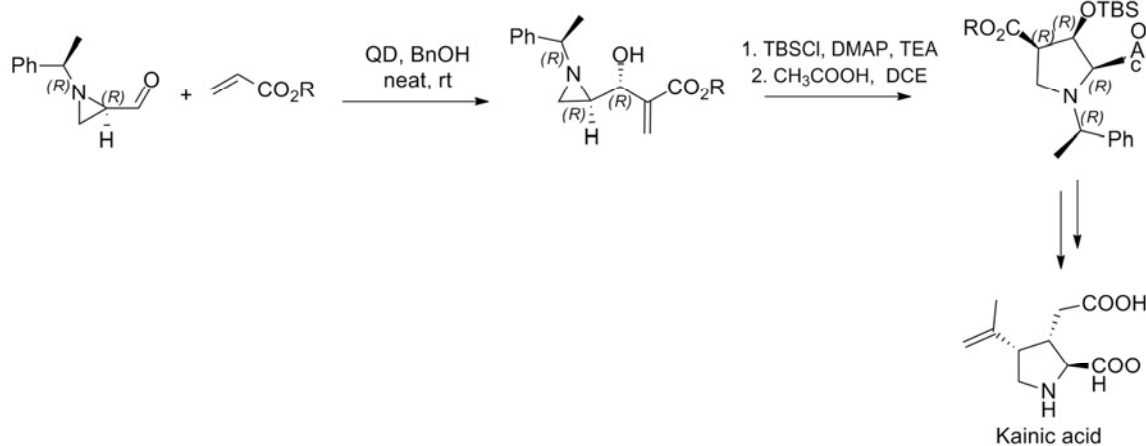
Morita-Baylis-Hilman reaction of chiral aziridine Aldehyde and distereo selective synthesis of 2,3,4-trisubstituted pyrrolidine

deepak singh, Jaedeok Lee¹, Hyun-Joon Ha^{1,*}

Chemistry, Hankuk University of Foreign Studies, Korea

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

The distereo selective MBH reaction of (*R*)-1-((*R*)-1-phenylethyl)aziridine-2-carbaldehyde was achieved in stereo selective manner with various alcohol as additive. The regio specific aziridin ring opening of MBH product by acetic acid yielded 2,3,4-trisubstituted pyrrolidine via aza Michael reaction, which may have utility for the synthesis of various biologically active compounds including Kainic acid.



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Type: Poster Presentation, Time: FRI 13:00~14:30

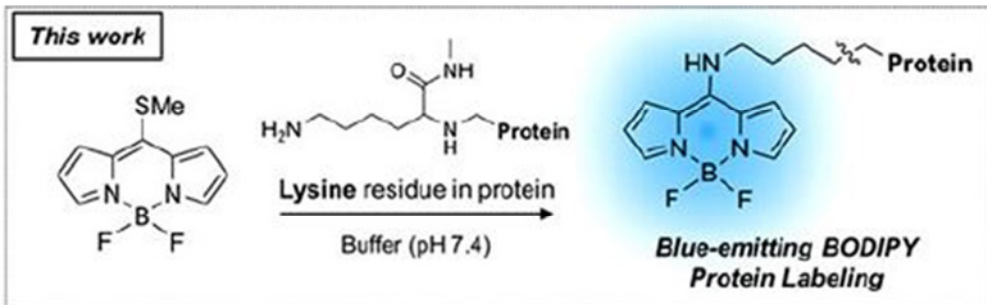
Fluorescent Labeling of Protein Using Blue-Emitting BODIPY Derivatives

Kyeong Hwan Kim, Kyo Han Ahn^{*}, Seo Won Cho, dokyoung kim¹

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

¹*College of Medicine, Kyung Hee University, Korea*

Labeling of biomolecules with a signaling unit is a crucial methodology for studying molecular interactions in biological systems.¹ A fluorescence-based labeling method has received great attention with remarkable progress in the development of new labeling chemistries. Researchers can monitor a specific components in a complex biological environment by labeling it with a fluorescent tag. So far several labeling chemistries such as click-chemistry, condensation reaction, ester/amide bond formation, and thiol-ene reaction have been reported.² Diverse fluorescent signaling units (called dyes) which cover from visible to near-infrared wavelength regions have been reported. However, in spite of its importance for studying the fluorescence resonance energy transfer from or to intrinsic biological fluorophores such as tryptophan and flavin adenine dinucleotide, the development of blue-emitting dye for protein labeling have been rarely explored. Even though a few coumarin-based blue-emitting dyes have been reported, these dyes have a shortcoming of environment-sensitive property: the emission properties of coumarin dyes, a class of donor-acceptor type dipolar dyes, are sensitive to environment changes such as viscosity, polarity, pH, and ion concentration. In terms of protein labeling, BODIPY dyes retain suitable properties such as compact size and insensitivity to environment; hence, dye labeling not only can causes minimal interference to protein activity but also can provide signals insensitive to the environment. Herein, we disclose 8-thiomethyl-BODIPY alleviates such issues, offering a novel blue tag for labeling of a protein with its activity retained.[1] M. Sameiro, T. Goncalves, Chem. Rev. 2009, 109, 190[2] X. Chen, Y.-W. Wu, Org. Biomol. Chem. 2016, 14, 5417



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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-388**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Control of Sequential Isomerization: Reactions of o-Lithiated Aryl Ethers in Flow

Hyune-Jea Lee, Heejin Kim¹, Juni-chi Yoshida^{1,*}, Dong Pyo Kim^{*}

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

¹*Department of Synthetic and Biological Chemistry, Kyoto University, Korea*

The control of isomerization is one of the significant issues in organic synthesis. In pharmaceutical industry area, flawless control of isomerization is important to not only curtail the work up process but also economically reduce the total pharmaceutical process cost. Especially in case of rapid and sequentially stepwise isomerization of reaction intermediates, controlling isomerization is still difficult or impossible to achieve by conventional flask reactions. Herein, we report the flow-assisted control of sequential isomerization of o-lithiated ethers using microreactors. The isomerization was sequentially proceeded by 1) intramolecular translocation and 2) [1,2]-Wittig-rearrangement. The reaction conditions for the generation and sequential isomerization of o-lithiated aryl ethers were optimized by controlling the residence time at room temperature. We also studied kinetic difference of reactions by changing the moieties of aryl ethers.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Ratiometric Fluorescence Detection System of Anthrax Biomarker using Eu^{III}-EDTA Functionalized Poly(diacetylene) Liposomes

Kyo Han Ahn^{*}, Ye Jin Reo

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

Bacillus anthracis is the pathogen of anthrax that can cause fatal infection in living organisms, including humans. The bacteria is able to form dormant endospores in which it can survive in any harsh conditions for a long time. However, the endospores become activated under favorable environmental conditions.1 Calcium dipicolinate (DPA, pyridine-2,6-dicarboxylate) is known as a major component of the bacterial endospores, being one of Anthrax Biomarker. Lanthanide ions have been used for detecting Anthrax biomarker due to a long lifetime, a sharp line-like luminescence spectrum, and a large Stokes shift.2 Herein, DPA acts as the antenna molecules of Lanthanide ions in order to prevent f-f transition.3 In addition, EDTA(ethylenediaminetetraacetic acid) is used as a chelating ligand for better signaling behavior. Thus, we report red color fluorescent PDA derived liposome dye containing Eu^{III}-EDTA complex which offers convenient, sensitive, and selective detection method for anthrax biomarker. References[1] a) K. A. Edwards, H. A. Clancy, A. J. Baumner, Anal. Bioanal. Chem. 2006, 384, 73. b) I. Lee, W. K. Oh, J. Jang, J. Hazard. Mater. 2013, 252, 186. c) L. M. Irenge, J. L. Gala, Appl. Microbiol. Biotechnol. 2012, 93, 1411. [2] a) B. Setlow, S. Atluri, R. Kitchel, K. Koziol-Dube, P. Setlow, J. Bacteriol. 2006, 188, 3740. b) D. L. Rosen, C. Sharpless, L. B. McGown, Anal. Chem. 1997, 69, 1082. [3] a) A. Thibon, V. C. Pierre, Anal. Bioanal. Chem. 2009, 394, 107. b) H. Seo, S. Singha, K. H. Ahn, Asian. J. Org. Chem., 2017, Just accepted manuscript

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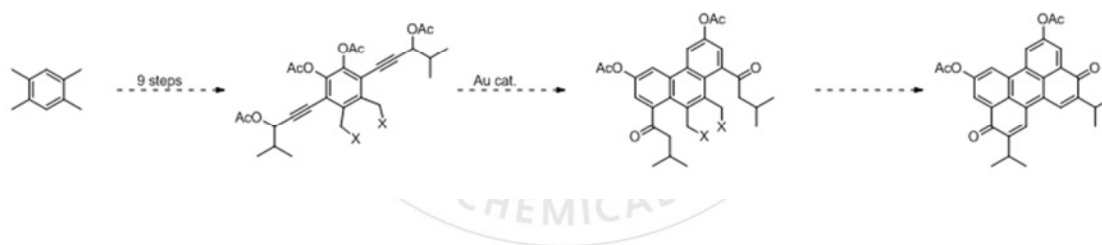
Type: Poster Presentation, Time: FRI 13:00~14:30

Extended Study on Multiple Cyclization by Gold Catalysis

Heo Hoongu, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

Our particular attention has been focused on Au-activated complexes of propargylic carboxylate. Also, we previously reported novel Gold-catalyzed cycloisomerizations. We have applied the reaction we had done to benzene including sets of 3-acetoxy-4-methylpent-1-yne to extend our study. We have tried to prepare substrate and make a multiringed compound based on the reaction.



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Type: Poster Presentation, Time: FRI 13:00~14:30

One-Flow Synthesis of Heterocyclic Thioquinazolinones through Serial Microreactions with Two Organolithium Intermediates

JiHo Kang, Hyune-Jea Lee, Heejin Kim¹, Dong Pyo Kim^{*}

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

¹*Department of Synthetic and Biological Chemistry, Kyoto University, Korea*

The synthesis of pharmaceutical compounds via short-lived intermediates in microreactor is attractive, because of the fast flow and high throughput. Additionally, intermediates can be utilized sequentially to efficiently build up a library in a short time. Various S-benzylic thioquinazolinone derivatives are synthesized within 10 s in high yields (75~98%) at room temperature. These three-step reactions involve two organolithium intermediates, an isothiocyanate-functionalized aryllithium intermediate, and a subsequent lithium thiolate intermediate.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A highly selective phosphorescence chemodosimeter based on Ir (III) complex for mercury (II) ion

Hayoung Rhee, JONG-IN HONG^{1,*}

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

Mercury, one of the most prevalent toxic metal elements, poses severe risks for human health and the environment. Thus, several molecular probes have been developed for the colorimetric and fluorometric detection of mercury. Nevertheless, it is still urgent to develop a rapid, selective and sensitive probe for mercury (II) ion. Herein, we report two Ir (III) complex-based phosphorescence chemodosimeters for the selective detection of mercury (II) ion. They show high selectivity and sensitivity to mercury ion (II) over other metal ions. Acetylacetonate ancillary ligand of the probe 1 reacts with mercury (II) ion selectively, inducing phosphorescence enhancement with concomitant blue-shift of the emission spectra. Meanwhile, mercury (II) ion selectively quenches the phosphorescence of the probe 2. The probe 1 and 2 showed low detection limit (LOD) as 73 nM and 202 nM, respectively. Details of synthesis, photophysical properties and sensing mechanism will be presented.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Higher Order Structures of Aromatic Helical Foldamers using Quadruple Hydrogen Bonding

Seungwon Lee, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

Recently, the tertiary, quaternary-like or bundled structures of foldamers which display unique functions have been growing as an important topic of research.¹ We herein have prepared indolocarbazole-pyridine hybrid foldamers that contain 2-ureido-4-pyrimidinone (UPy) quadruple hydrogen-bonding moieties in the aromatic backbone side chains. In non-polar solvents, the UPy-containing synthetic oligomers not only fold into a helical conformation but also afford the self-assembled higher ordered structures. The folding and self-assemblies of the foldamers have been revealed by ¹H NMR and VPO experiments. Details including the synthesis and characterization of oligomer and assemblies will be described in the presentation. .References(1)(a) Delsuc, N.; Massip, S.; Leger, J. M.; Kauffmann, B.; Huc, I. J. Am. Chem. Soc. 2011, 133, 3165–3172. (b) Collie, G. W.; Bailly, R.; Pulka-Ziach, K.; Lombardo, C. M.; Mauran, L.; Taib-Maabar, N.; Dessolin, J.; Mackereth, C. D.; Guichard, G. J. Am. Chem. Soc. 2017, 139, 6017-6276.

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Type: Poster Presentation, Time: FRI 13:00~14:30

Regiodivergent C–H Alkenylation of Pyrazoles

HyunTae Kim, Jung Min Joo^{*}, Changhoon Shin¹

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¹*department of chemistry, Pusan National University, Korea*

Pyrazole is one of the most important heterocycles in drug discovery. It can be functionalized by either electrophilic aromatic substitution at the nucleophilic C4 position or strong-base-mediated substitution at the C5 position, which possesses the most acidic C–H bond. However, the transition-metal-catalyzed C–H functionalization has not yet been able to take advantage of the electronically and sterically different nature of these C–H bonds at the C4 and C5 positions. In this work, we have developed palladium-catalyzed regioselective C4- and C5-alkenylation of pyrazoles. A variety of alkenes including acrylate, acrylamide, and styrene derivatives, and vinyl derivatives could be installed at the C4 and C5 positions of pyrazoles. Kinetic isotope effects and H/D exchange experiments were performed in order to obtain mechanistic insights into C4- and C5-alkenylation. Furthermore, C5-alkenyl pyrazoles were useful for the preparation of 3-alkenyl pyrazoles that are not easily accessible by C–H alkenylation.

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Microwave Assisted N-Alkylation of 1-Deoxynojirimycin

JAEHYUN KIM, Woonsang Hwang, Kooyeon Lee*

Department of Bio-Health Technology, Kangwon National University, Korea

N-Substituted deoxynojirimycin derivatives are an important class of molecules in medicinal chemistry and drug discovery. In this studies, a fast and facile method for preparation of N-alkylated deoxynojirimycin(DNJ) under microwave irradiation is presented. The microwaves remarkably accelerated these N-alkylations, the reaction times decreased dramatically. Consequently, the microwave assisted alkylation of N-containing sugars could be considered eco-friendly. Mostly, under MW irradiation the yields are also higher. A comparative study of microwave vs. classical conditions has been done. Thus, based on the results of this study, various N-alkylated DNJ derivatives can be synthesized easily and quickly. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (No. 2015H1C1A1035955).

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Development of Blue Thermally Activated Delayed Fluorescence Emitters Using Triphenylamine Electron Donor

Youngnam Lee, JONG-IN HONG*

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 (T1) to the singlet state (S1). 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 donor-acceptor blue TADF emitters using triphenylamine as an electron donating group and quinoxaline (1)/quinazoline (2) as electron accepting groups. They were synthesized by Suzuki-Miyaura coupling as a key step and exhibited well separated HOMO and LUMO by twisted molecular conformation inducing TADF. Furthermore, these molecules have wide band gap of 3.06 and 3.10 eV for (1) and (2), respectively. Details of synthesis, photophysical properties and device properties will be presented.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Highly sensitive Electrogenerated chemiluminescence probe for hydrogen sulfide based on Cyclometalated Ir(III) Complex

Joonho Park, JONG-IN HONG^{1,*}

Department of Chemistry, Seoul National University, Korea

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

Hydrogen sulfide (H₂S) has been known as a toxic gas with unpleasant rotten egg smell, however it is now recognized as an important biological regulator and signaling molecule in many physiological processes and diseases. It is important, therefore, to understand the role of H₂S in biological samples, which has remained challenging due to limited methods for detecting endogenous H₂S. Recently, the use of electrogenerated chemiluminescence (ECL) has increased a lot of interests due to their advantages such as high sensitivity, wide linear response range, good reproducibility and simple analytical process. Herein, we introduce a new ECL chemodosimetric probe for H₂S based on cyclometalated Ir(III) complexes. Probe 1 has azido methyl benzoyl moiety as a reaction site on the main ligand. It exploits the reduction of azide to its parent amine by H₂S, which leads to cascade reaction of intramolecular cyclization cleavage. These systems show a good ratiometric PL property and “turn-off” ECL sensing property. Details of synthesis and photophysical studies will be presented.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Triethylborane-mediated radical addition reaction for synthesis of 3-substitued isoindolinone derivatives on water

TAE KYU NAM, Doo OK JANG *

Department of Chemistry, Yonsei University, Korea

Water is a sustainable and environmentally benign solvent. It is cheap, readily available, non-flammable, and non-toxic. In addition, water influences significantly polar reactions with specific interactions such as polar, hydrophobic, trans-phase, and hydrogen bonding interactions. However, the solvent effect is known to be negligible in radical reactions. Thus, water was employed as a reaction medium for radical reactions with no expecting the solvent effect. In this context, research efforts on radical reactions employing water were towards increasing the solubility of reactants and initiators. Herein, we wish to report a radical addition reaction to C=N bond "on water" at room temperature for the synthesis of 3-substitued isoindolinone derivatives. In the course of the research, a significant solvent effect was observed. The advantages of the present process includes high yield, using green solvent, and easy work-up process.

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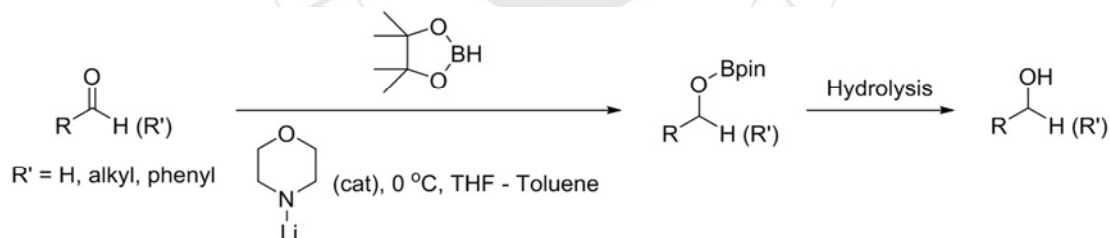
Type: Poster Presentation, Time: FRI 13:00~14:30

New catalytic hydroboration of aldehydes and ketones using pinacolborane and lithium morpholide as catalyst

Hyun Tae Kim, won kyu sin, Duk Keun An^{*}

Department of Chemistry, Kangwon National University, Korea

Hydroboration of various functional groups is broadly used in organic synthetic fields. And, catalytic version of hydroboration actively studied. Recently, we found the new catalytic hydroboration of aldehydes and ketones using pinacolborane and a catalytic amount of lithium morpholide in excellent yields under mild reaction condition. Furthermore, we plan to use various secondary amines including sterically crowded amines for selective reduction.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Dendritic Multichromophores: Aggregation-Enhanced and Unusually Blue-Shifted Emission

Dae Ho Hong, Suk-il Kang¹, Dongwhan Lee^{1,*}

Department of chemistry, University of Florida, United States

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

Using a tris(triazolo)benzene-based polyheteroaromatic molecular platform, we have constructed a series of dendritic donor-acceptor chromophores. A cross-conjugated nature of these constructs leads to an effective electronic “decoupling” between branching units, which greatly simplified our theoretical/computational studies to understand structure-dependent photophysical properties. Moreover, a systematic expansion in the dendritic pattern correlates nicely with an increasing molecular surface area, which induced the formation of solution aggregates in mixed solvents. A combination of fluorescence measurements, DLS, SEM, and TEM studies point toward the formation of submicron-sized molecular aggregates that display blue-shifted emission with enhanced intensity. In this presentation will be discussed our interpretation of this unusual behavior and its implications for the rational design of solid-state emitters.

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Effective synthesis of homoprotoberberine analogs

Yuri CHoi, Gangadhar Rao Mathi¹, Seulgi Kim¹, Jong Yeon Hwang¹, PILHO KIM^{1,*}, Sung Yun Cho²

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

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

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

The synthesis of tetrahydroisoquinoline containing natural products, such as methopholine and homoprotoberberine, have been one of the major topics of medicinal and organic chemists due to their intriguing biological activities. Recently, we developed a novel synthetic methodology facilitating one-pot double addition of alkyl halides on 1-methyl-3,4-dihydroisoquinoline, which was also applicable for the synthesis of methopholine in just two steps from a dihydroisoquinoline. In the context of application of double addition chemistry, homoprotoberberine analogs were prepared through intramolecular double addition of alkyl halides on 1-methyl-3,4-dihydroisoquinoline. The scope and limitation of this chemistry will be discussed.

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Code: **ORGN.P-402**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

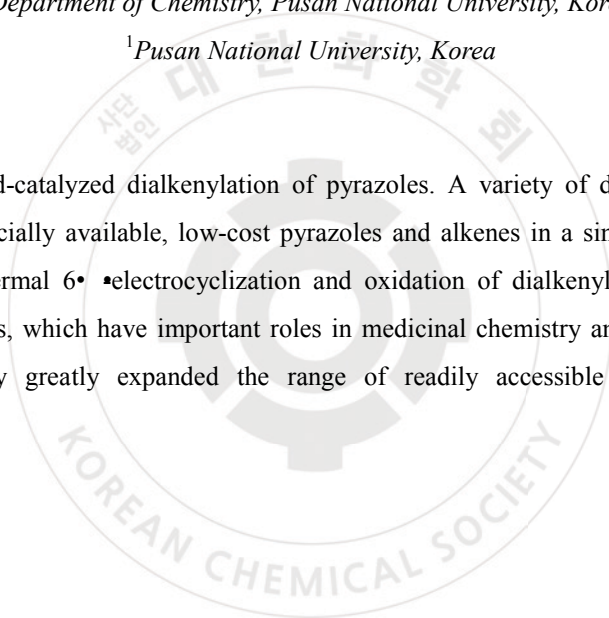
Synthesis of Indazoles by C–H Alkenylation of Pyrazoles

Geunhee Kang, YEJI HWANG, Jin Hyeok Jang¹, Jung Min Joo^{*}

Department of Chemistry, Pusan National University, Korea

¹*Pusan National University, Korea*

We have developed Pd-catalyzed dialkenylation of pyrazoles. A variety of dialkenyl pyrazoles were prepared from commercially available, low-cost pyrazoles and alkenes in a single step. Furthermore, a sequence involving thermal 6 π -electrocyclization and oxidation of dialkenylated pyrazoles provided functionalized indazoles, which have important roles in medicinal chemistry and material science. This comprehensive strategy greatly expanded the range of readily accessible pyrazole and indazole derivatives.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-403**

Area: Organic Chemistry

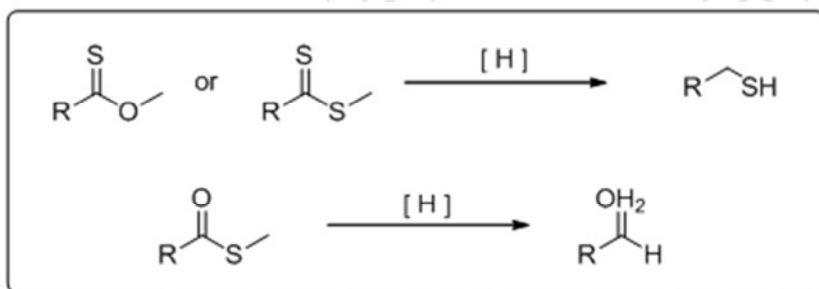
Type: Poster Presentation, Time: FRI 13:00~14:30

Reduction of S-methyl thioate, O-methyl thioate and methyl thioate

Da Hun Ma, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Recently, we reported that new reducing agents for the reduction of various ester. As a part of our research program, we decided to attempt the reduction of S-methyl thioates, O-methyl thioates and methyl dithioates. We previously carried out the reduction of S-methyl benzothioate, O-methyl benzothioate and methyl benzodithioate. As a result, O-methyl benzothioate and methyl benzodithioate were observed to smoothly undergo conversion to the corresponding thiol in quantitative yields. However, in the case of S-methyl benzothioate gave the corresponding aldehyde in very good yield. Furthermore, we are studying to know the reason using density functional theory (DFT) calculation.



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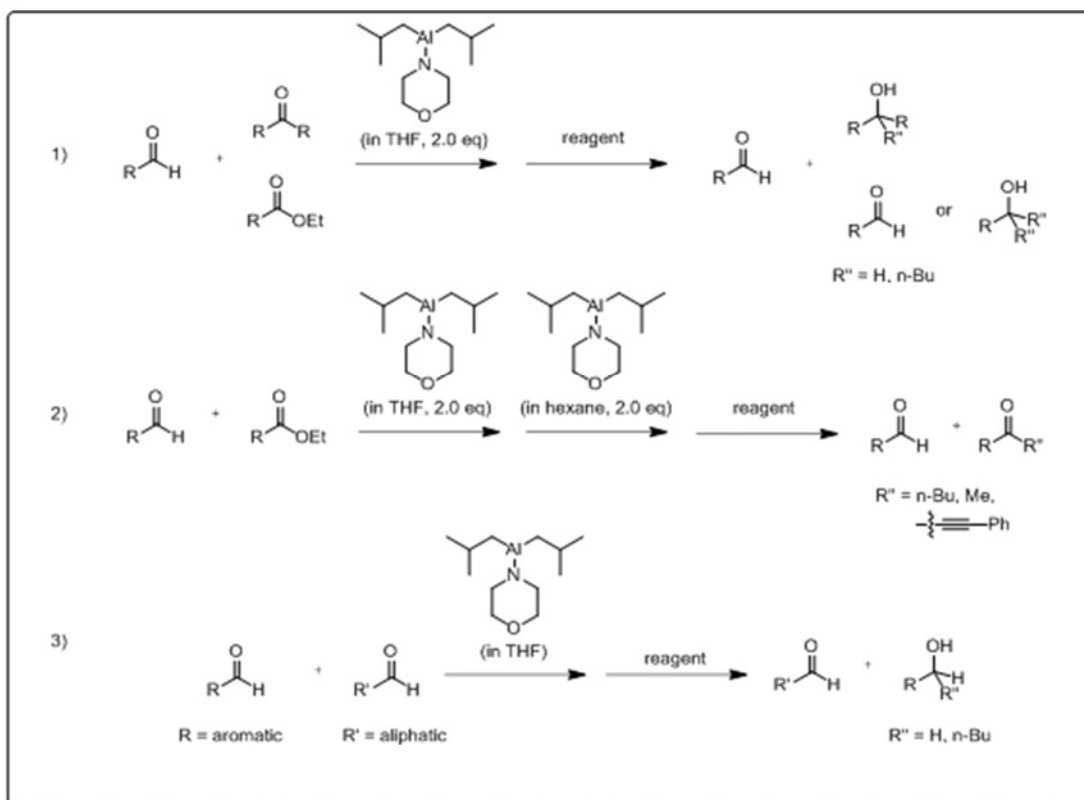
Type: Poster Presentation, Time: FRI 13:00~14:30

Chemoselective transformation of carbonyl compounds using new in situ protecting method with diisobutyl(morpholino)aluminum

won kyu sin, Sujin Seo, Duk Keun An *

Department of Chemistry, Kangwon National University, Korea

Chemoselective reaction is one of the important organic synthetic methods that is expected to be widely used for the synthesis of complex natural products showing significant biological activity and other useful materials. Chemoselective transformation studies have been generally reported using protection/deprotection and in situ protecting(masking/demasking) method. Recently, we found that possibility of new in situ protection of aldehydes using synthesized diisobutyl(morpholino)aluminum from DIBALH(in THF) and morpholine. In order to investigate the in situ protection ability of diisobutyl(morpholino)aluminum, we progressed the reaction of aldehydes and carboxylic acid derivatives. As a result, diisobutyl(morpholino)aluminum is used as in situ protecting agent of aldehyde and carboxylic acid derivatives is reacted with added reducing agents or alkyllithium to become aldehyde, ketone or alcohol. Furthermore, when exist to both aromatic and aliphatic aldehyde, this reagent had high selectivity for aliphatic aldehyde in the presence of aromatic aldehyde and remained substrate is converted to alcohol from reaction of reducing agents or alkyllithium.



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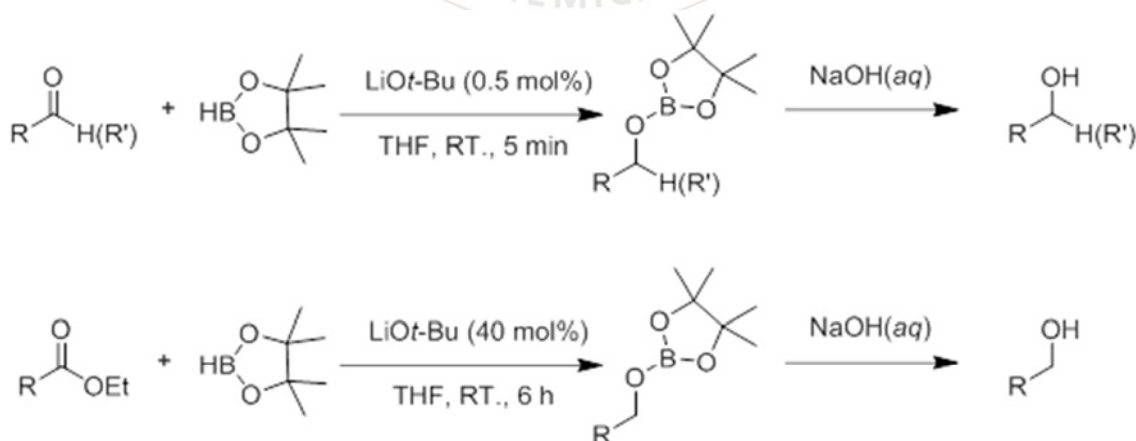
Type: Poster Presentation, Time: FRI 13:00~14:30

New and Efficient Catalytic Hydroboration of Carbonyl Compounds with Pinacolborane and Lithium t-Butoxide as Catalyst

jea ho Kim, won kyu sin, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

The reduction is one of the most fundamental tools in the organic synthesis. And hydroboration of carbonyl compounds is a very useful technique to make alcohols, this type of reduction has been studied for a long time. And many kinds of catalytic hydroboration using various metal catalyst have been reported. Among them, Clark and co-workers recently reported catalytic hydroboration of a ketone with pinacolborane and NaOt-Bu (5 mol%) in 86~93% yields. We wish to explore for improving the reactivity and selectivity through change the metal alkoxide having different counter cation such as LiOt-Bu or KOt-Bu. We have developed a facile and alternative new catalytic hydroboration method of aldehyde and ketone using pinacolborane and lithium t-butoxide in very good yields under mild reaction condition.



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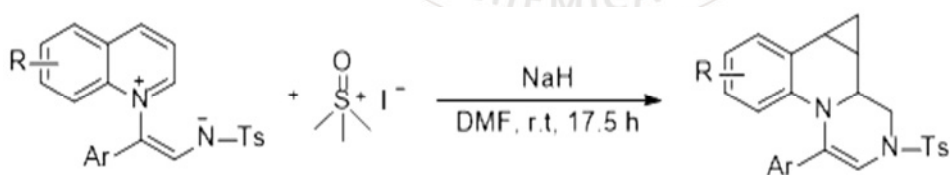
Type: Poster Presentation, Time: FRI 13:00~14:30

Metal-free cascade [2+1]/[5+1]-cycloaddition: Synthesis of cyclopropane-fused pyrazino-quinolines

Donguk Ko, Jiyoun Lee, Eun Jeong Yoo*

Department of Chemistry, Kangwon National University, Korea

Cyclopropane ring is one of the unique structural units present in wide range of natural and synthetic compounds exhibiting biological and pharmaceutical activity, such as natural products (\pm)-Echinopines and (-)-crispatene possess fused cyclopropane skeleton. Due to high angle strain (28 Kcal/mol) the synthesis of cyclopropane containing compounds, specially fused-cyclopropanes are challenging task. Recently, our group discovered that the pyridinium-zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners. In this symposium we will disclose a new metal-free cascade [2+1]/[5+1] cycloaddition reaction of analogous quinolinium-zwitterion with 1C coupling partners to form cyclopropane fused heterocyclic compounds.



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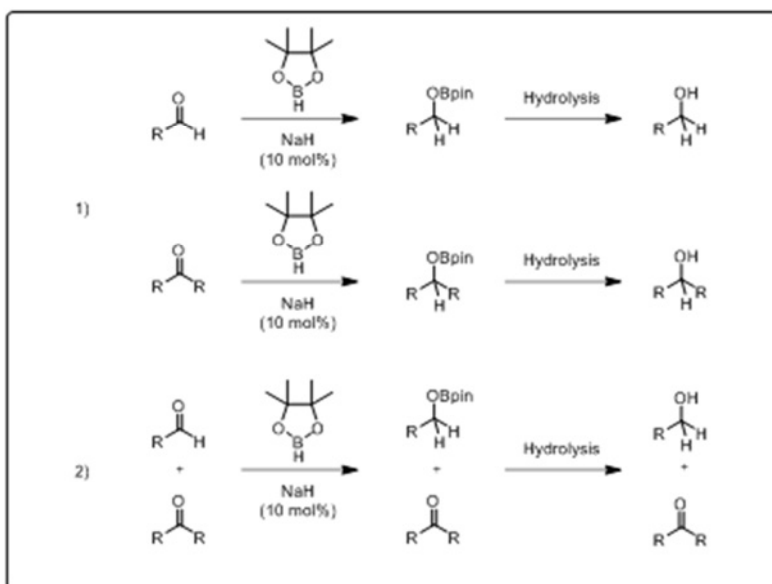
Type: Poster Presentation, Time: FRI 13:00~14:30

New chemoselective hydroboration with pinacolborane and NaH as catalyst

Hanbi kim, won kyu sin, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

The hydroboration of aldehydes and ketones is one of the useful reaction in organic synthesis. Borane reducing agents such as NaBH₄ and BH₃ have been utilized for the stoichiometric hydroboration of aldehydes and ketones. And, catalytic hydroboration of carbonyl compounds have been recently studied. Catalytic hydroboration of aldehydes and ketones using transition-metal(Rh, Ru, Mo, Ti, Cu, Zn, etc.), main-metal(Li, Na, K, Mg, Al, Ge, etc.) and non-metal(P) is well known. Recently, we found the new method of catalytic hydroboration using pinacolborane and catalytic amount of NaH. This new method provides hydroboration of aldehyde and ketone both in excellent yields under mild reaction conditions. Furthermore, this method has the potential for the chemoselective reduction of aldehydes in the presence of ketones.



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Area: Organic Chemistry

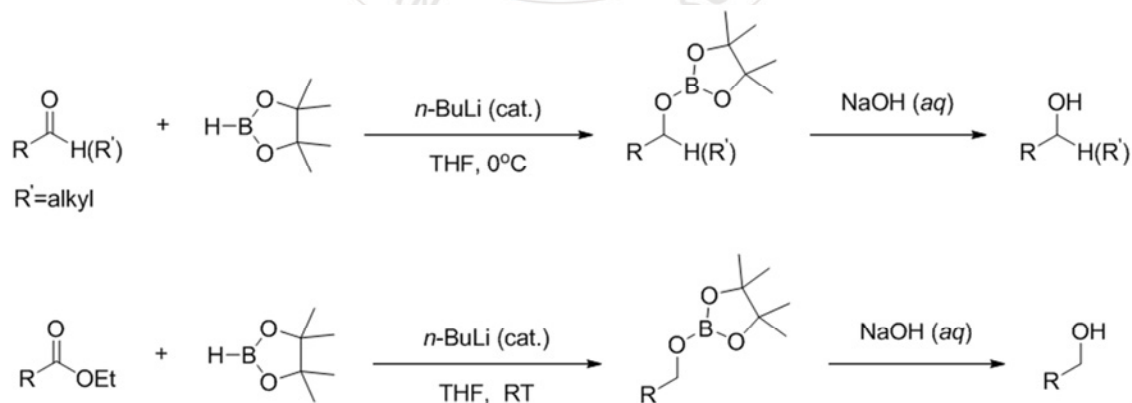
Type: Poster Presentation, Time: FRI 13:00~14:30

Study of New Catalytic Hydroboration with Representative Carbonyl Compound Using Pinacolborane and n-Butyllithium as Catalyst

SuJin Yang, won kyu sin, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Hydroboration is one of the important and useful reaction in organic synthesis. And, various catalytic hydroboration of aldehydes and ketones using many kind of metal catalysts such as V, Mn, Zn and Pd have been reported. On the other hand, catalytic hydroboration of esters only reported that using Mg-complex catalyst. Recently, we investigated new catalytic hydroboration method of aldehydes, ketones and esters by treatment with pinacolborane and catalytic amount of n-Butyllithium under mild reaction condition. Furthermore, we plan to use various organometallic catalysts such as various alkyl lithium and Grignard reagents in this reaction.



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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-409**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Safer Synthesis of Tetrazoles from Secondary Amines using Trichloroacetonitrile

su-jin Oh, Yeong-Gweon Lim^{*}

4-2, Agency for Defense Development, Korea

Tetrazole which are aromatic heterocyclic compounds with high nitrogen contents have been considered as promising building block of HIEMs (High-performance Insensitive Energetic Materials) due to their high heat of formation, high stability and environmentally friendly property. A new method for synthesizing the tetrazole derivatives from secondary amines through cyanation/tetrazolation has been developed by us. Trichloroacetonitrile is used as a cyano source to synthesize N-nitrile instead of highly toxic and expensive cyanogen bromide. In this protocol, secondary amines with various substituted groups proceed smoothly, and the desired tetrazole derivatives are obtained directly in good to high yields without isolation of intermediate cyanamides.

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Area: Organic Chemistry

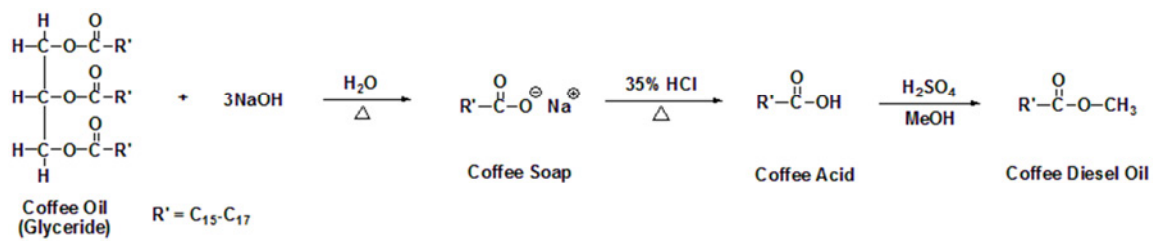
Type: Poster Presentation, Time: FRI 13:00~14:30

Effective stepwise conversion of spent coffee grounds for biodiesel production

kyung-min choi, Eun-ji Sa, vaidya raghavenderrao, Kalpesh Patil, Dong-Soo Shin*

Department of Chemistry, Changwon National University, Korea

Spent coffee grounds are attractive source for biodiesel production due to their high content contain ~15% triglycerides by dry weight, which can be converted to biodiesel using various transesterification methods. But low contents of biodiesel after transesterification of coffee oil extracted with spent coffee grounds have many problems. We attempted stepwise reactions that coffee oil has been converted by saponification and acidification follows esterification for high contents of biodiesel. In addition GC-MS analysis showed the presence of C16-C18 methyl esters of fatty acids can be consisted with saturated and unsaturated methyl esters which contains methyl esters of palmitic acid, linoleic acid, and stearic acid.



Palmitic Acid ethyl ester



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Area: Organic Chemistry

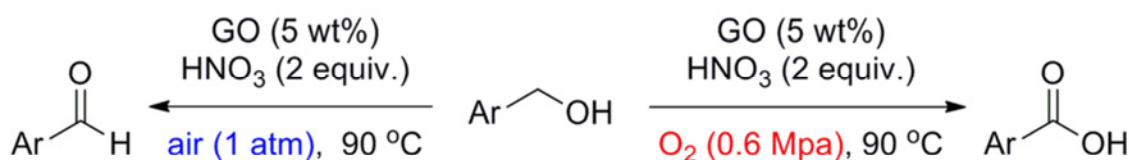
Type: Poster Presentation, Time: FRI 13:00~14:30

Impact of Carboxyl Groups in Graphene Oxide on Chemoselective Alcohol Oxidation with Ultra-Low Carbocatalyst Loading

TaeWoo Lee, Jung Woon Yang*

Department of Energy Science, Sungkyunkwan University, Korea

A highly efficient and simple chemoselective aerobic oxidation of primary alcohols to either aldehydes or carboxylic acids in the presence of nitric acid was developed, utilising 5 wt% graphene oxide as a carbocatalyst under ambient reaction conditions. Carboxylic acid functional groups on graphene oxides played a vital role in carbocatalyst activity, greatly influencing both the reactivity and selectivity. We also applied this protocol to a variant of the Knoevenagel condensation for primary alcohols and malonates with a secondary amine co-catalyst via cooperative catalysis.



- High chemoselectivity of the products
- Ultra-low carbocatalyst loading (5 wt%)
- High recyclability of graphene oxide

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Code: **ORGN.P-412**

Area: Organic Chemistry

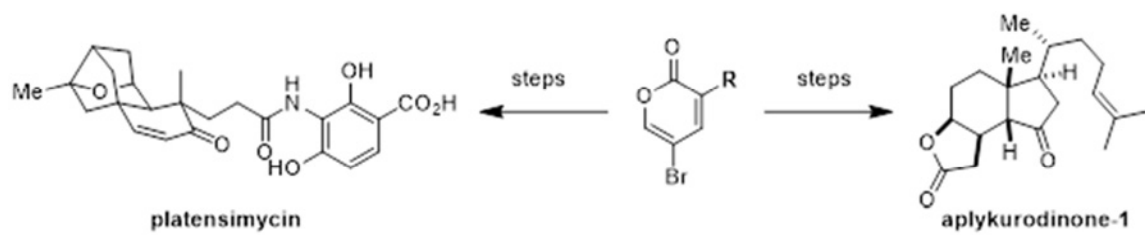
Type: Poster Presentation, Time: FRI 13:00~14:30

Intramolecular 2-pyrone Diels-Alder reactions towards asymmetric total syntheses of (+)-aplykurodinone-1 and (-)-platensimycin

Joon Ho Lee, Hyo mi Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Center for New Directions in Organic Synthesis, Department of Chemistry, Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul 04763, Korea During the past years, we have explored the Diels-Alder chemistry of 3,5-dibromo-2-pyrone as a new enophile synthon. Its synthetic versatility has been further exuberated by the recent discovery that either of the two C-Br groups can be selectively functionalized through transition metal catalyzed coupling reactions. The resultant 3- or 5-substituted 2-pyrones are also potent neutral dienes, and can undergo cycloaddition reaction to afford an array of densely functionalized cyclohexenes. Ever since then, we have explored the potential applicability of the rich chemistry embedded in the 2-pyrone cycloadducts, toward the synthesis of complex bioactive natural products. Recently, we began to prove the effectiveness of our concept by achieving successful total syntheses of a few natural products including trans-dihydronarciclasine, joubertinamine, mesembrine, crinine, crinamine, galanthamine, aspidospermidine, pancratistatin, 1-deoxylycorine, and lycorine. In conjunction to our continuous efforts toward target-oriented synthesis, we have devised a new synthetic route to (-)-neocosmosin A by way of an intramolecular Diels-Alder cycloaddition of 2-pyrone containing a bromopropiolate group as dienophile. In this elaboration, the IMDA reaction was accompanied by cycloreversion of carbon dioxide to give benzannulated macrolide with two bromide groups at C14 and C16. Installation of the pinacolboron groups and oxidations allowed completion of the total synthesis of (-)-neocosmosin A. Prompted by the effectiveness, we have further extended the 2-pyrone IMDA cycloaddition strategy to the total syntheses of (+)-aplykurodinone-1 and (-)-platensimycin. Our recent efforts in this line of chemistry will be presented.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Asymmetric total syntheses of (+)-aspidospermidine and (-)-tabersonine via regio-controlled Fischer indole synthesis

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Department of Chemistry, Hanyang University, Korea

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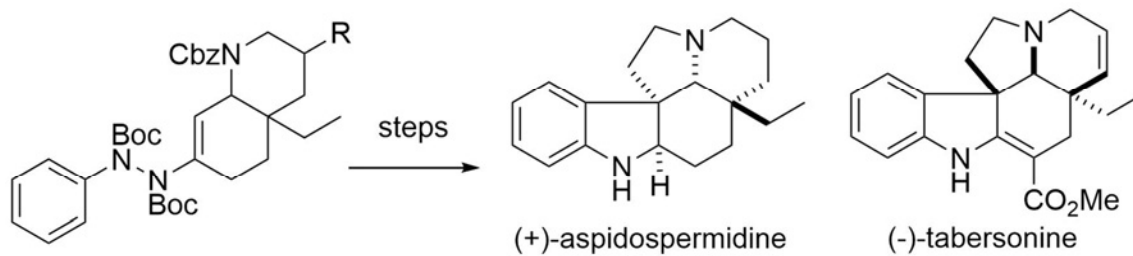
Recently we have demonstrated that ene-hydrazide readily available from enol triflate in regiochemically defined form may undergo Fischer indolization reaction with no regiochemical scrambling.¹ In order to prove its usefulness, we applied our new method to the syntheses of various aspidosperma alkaloids. The aspidosperma family comprises the largest group of indole alkaloids, with more than 250 compounds. The structural challenge posed by these alkaloids in conjunction with the potent pharmacological properties exhibited by several members has stimulated considerable effort directed toward their synthesis.² Prior to the synthesis of intricate aspidosperma alkaloids, we initiated the synthesis of (+)-aspidospermidine, the most popular aspidosperma alkaloid often used as testbed to evaluate effectiveness of new synthetic methods and/or routes. In our new approach, a base-catalyzed intramolecular aza-Michael reaction, in situ trapping of the resulting enolate, and subsequent C-N coupling with phenyl hydrazide afforded the key ene-hydrazides in high overall yields. Subsequent regioselective Fischer indolization under Lewis acidic conditions culminated in the synthesis of (+)-aspidospermidine. The same approach proved to be also effective for the synthesis of (-)-tabersonine. Presented herein are the details of the total syntheses of (+)-aspidospermidine and (-)-tabersonine.

Acknowledgement

This work was supported by a grant from the National Research Foundation of Korea (2014R1A5A1011165, Center for New Directions in Organic Synthesis).

References

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Venue: Kimdaejung Convention Center, Gwangju

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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Intramolecular Fischer indole synthesis towards the total synthesis of (+)-decursivine

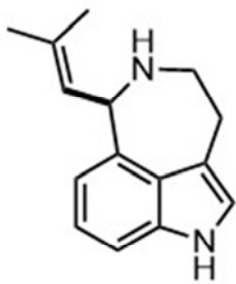
Dong-Hyun Kim, JEONGHWA Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

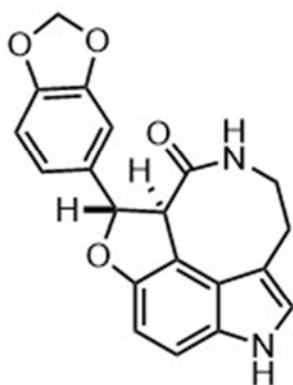
We have previously demonstrated that aryl hydrazides are effective surrogates of aryl hydrazines, undergoing various reactions including the Fischer indole synthesis to afford the corresponding indoles, when treated with enolizable aldehydes and ketones in the presence of an acid. Unlike aryl hydrazines,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

References

1. Park, J.; Kim, D.-H.; Cho, C.-G., *Org. Lett.* 2016, 18, 5098.
2. Park, J.; Kim, S.-Y.; Kim, J.-E.; Cho, C.-G., *Org. Lett.* 2014, 16, 178.
3. Park, I.-K.; Park, J.; Cho, C.-G. *Angew. Chem. Int. Ed.* 2012, 51, 2496.



(-)-aurantioclavine



(+)-decursivine



Conference Date: October 18~20, 2017

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Area: Organic Chemistry

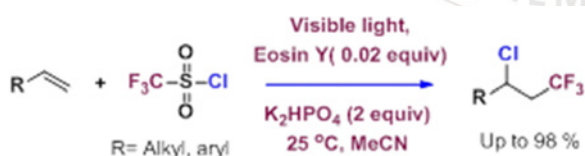
Type: Poster Presentation, Time: FRI 13:00~14:30

Visible light mediated chlorotrifluoromethylation with CF₃SO₂Cl by Eosin Y

vaidya raghavenderrao, Dong-Soo Shin^{*}, Kalpesh Patil

Department of Chemistry, Changwon National University, Korea

Photocatalytic reactions are interesting and lots of advantage like easy to access functionality of many functional organic molecules by irradiating the light, eco-friendly approach. Still many laboratories are using transition metal catalysts such as iridium, ruthenium, and platinum however they are expensive and could affect the efficiency of electronic materials while synthesizing it. We have been interested in Eosin Y because it is cheaper, efficient and it can be reacted in mild conditions give higher yields. Eosin Y, an organic dye, we are using that for photo catalytic reactions it'll produce single electron transfer (SET) rapidly so that radicals can be reacted, step by step. Based on this concept developed a new photocatalytic chlorotrifluoromethylation method with CF₃SO₂Cl by Eosin Y.



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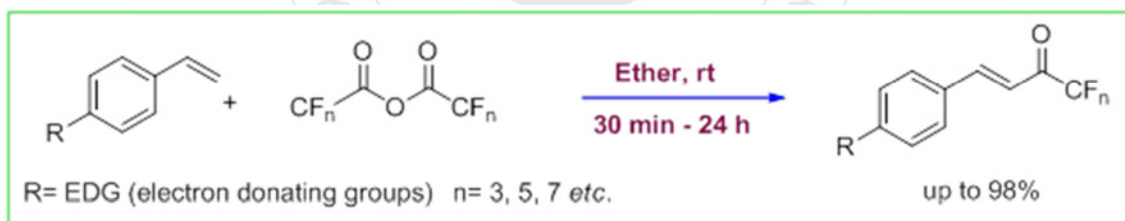
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of Perfluorostyryl ketones from styrenes

vaidya raghavenderrao, Dong-Soo Shin^{*}, Kalpesh Patil, Eun-ji Sa

Department of Chemistry, Changwon National University, Korea

A new route for synthesizing stereoselective one-pot synthesis of (E)-styrylperfluoroketones from styrenes by using trifluoro-, pentafluoro-, heptafluoro-acetic anhydrides. Majorly this protocol is working on electron donating group substituted styrenes and those are reacting with perfluoro anhydrides without addition of any base due to electron donating groups are giving driving force for self-mechanism to accelerate the reaction. Generally perfluorostyryl ketones are very difficult to produce, for example, Aldol condensation by using aldehydes in basic conditions.



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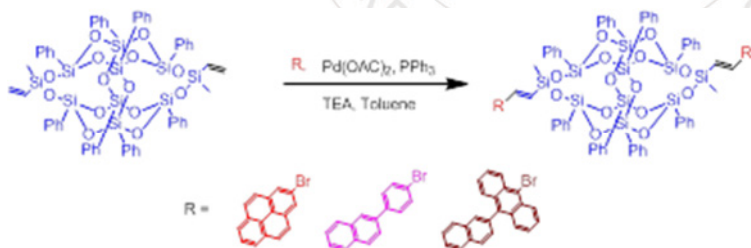
Type: Poster Presentation, Time: FRI 13:00~14:30

Design and synthesis of photoluminescence compound from Double-decker silsesquioxanes (DDSQ)

Kalpesh Patil, Dong-Soo Shin^{*}, vaidya raghavenderrao

Department of Chemistry, Changwon National University, Korea

DDSQ (double-decker-shaped silsesquioxane) is the one of the excellent organic-inorganic hybrid material to enhance the physical properties such as chemical, thermal and mechanical stability. Also DDSQ provide symmetrical cage like structure for fascinate to bind organic fluorescent compounds. We successfully synthesized three different type of compound by Heck reaction of DDSQ with 1-bromopyrene, 2-(4-bromophenyl) naphthalene and 9-(bromo-10-(naphthalene-2-yl)anthracene. These compound has excellent photo-luminescence activity, it may use as OLED application.



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Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electronic Effects on the Substituted, Antiaromatic Naphthorosarins; Journey to the Synthesis of the Key Building Blocks

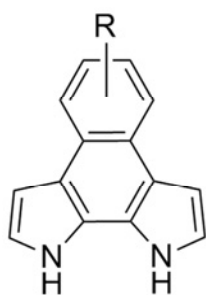
Dikhi Firmansyah, Yoorim Go, Jinhee Bae¹, Hye Ryung Byon^{2,*}, Chang Hee Lee^{*}

Department of Chemistry, Kangwon National University, Korea

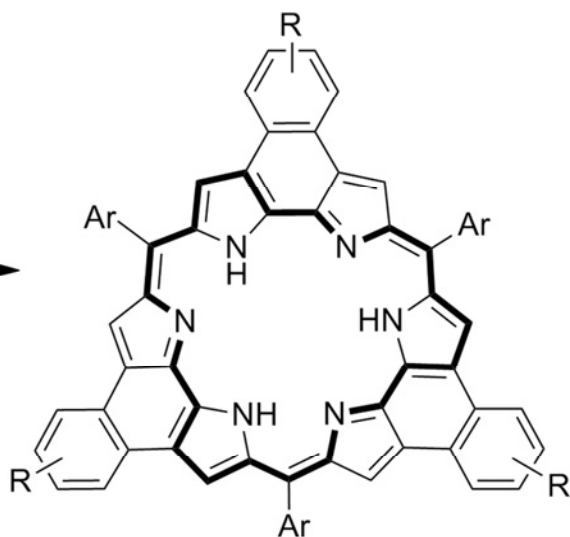
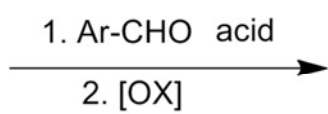
¹*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

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

Annulated rosarin, β , β' -two-carbon bridged-(1.0. 1.0. 1.0) hexaphyrin derivatives, which are 24 π -antiaromatic compounds, are known to form stable one-electron reduced species upon protonation. However, the syntheses of the key building block, naphthobipyrrole were somehow hurdled due to the limited accessibility of the building blocks. The only reported synthetic method for the naphthobipyrrole is through the Fisher-Indole synthesis. Several attempted synthesis of naphthobipyrrole through oxidative coupling of dipyrrolylbenzene derivatives were not successful due to unexpected side reactions such as polymerization. With this presentation, we report the synthesis of two new 5,6-substituted naphthobipyrroles (namely fluoro substituted and methyl substituted) with overall synthetic yields of over 40%. The synthesis of corresponding rosarin analogues using synthesized building blocks were successful with the yield of ranging from trace to 24%. The 5,6-difluoro substituted building block afforded 24% yield of corresponding rosarin. However, the 5,6-dimethyl substituted one gave only trace amount of desired rosarin. The time-dependent spectral changes after addition of excess acids (HCl and HI⁻) indicate that the single electron reduction are faster in fluoro-substituted rosarin. Slightly increased reduction potential is ascribed to the electron withdrawing effect of fluorine atoms. Detailed studies on the synthesis and electrochemical data will be presented.



R = H, F, Me



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Area: Organic Chemistry

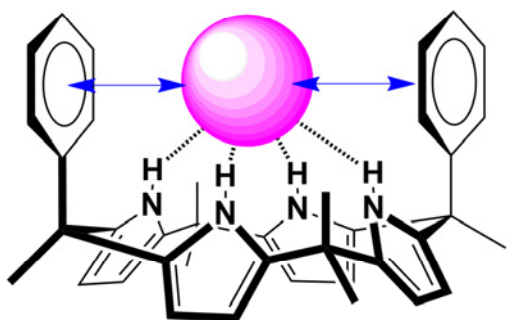
Type: Poster Presentation, Time: FRI 13:00~14:30

Nature of halide recognition modes in meso-phenylethynyl picket calix[4]pyrrole

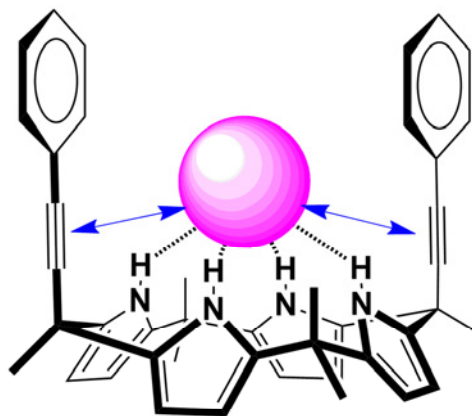
ranjan dutta, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

Supramolecular chemistry is a vibrant field exploring the realm of non-covalent interactions, providing a base for highly specific recognition, transport, and regulation events triggering numerous biological processes. Calix[4]pyrroles have been studied extensively as effective receptors for anions, ion-pairs and efficient anion transporter through lipophilic membranes. We have been interested in the investigation of anion binding properties of calix[4]pyrrole bearing aryl groups on the diametrical meso-positions with cis-configuration. As shown in figure 1 CP-1 has directly attached aryl groups while triple bonds are inserted between the meso-carbons and the aryl groups in case of newly synthesized receptor CP-2. Comparative anion binding properties of CP-1 and CP-2 are investigated by various spectroscopic techniques to understand the effect of pi-extension. Significant enhancements in the halide binding affinities for CP-2 over CP-1 are observed from ITC measurements. Presence of attractive CH-anion interactions are attributed to the observed higher anion binding affinity for CP-2 as inferred for ¹H-NMR titration study, while repulsive anion-pi interaction is responsible for lower binding affinity for CP-1. It is noteworthy to mention that cavity binding of halides is previously reported for CP-1. Finally unambiguous confirmation of anion binding is established from X-ray structural analysis of the chloride-complex of CP-2 where cup side binding of chloride is observed. Comparative anion binding properties and structure-property relationship for the ethynyl extended system will be presented in details.



CP-1



CP-2



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Code: **ORGN.P-420**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Anion Dependent Binding Mode Changes in meso-(5,6-Dichlorobenzimidazole)-picket Calix[4]pyrrole

endale mulugeta, ranjan dutta, Qing He¹, Vince Lynch¹, Jonathan Sessler¹, Chang Hee Lee^{*}

Department of Chemistry, Kangwon National University, Korea

¹*Chemistry, University of Texas, Austin, United States*

A deep-cavity calix[4]pyrrole anion receptor bearing 5,6-dichlorobenzimidazole subunits at the diametrically opposed meso-positions has been synthesized and fully characterized. Anion binding properties of the receptor studied by ¹H NMR spectroscopy indicate that the synthesized receptor exhibits higher affinity for the fluoride anion over the chloride anion with high discrimination factor. The analysis of the solid state structures of the complexes show significant differences in the geometries between fluoride complex and chloride complex. The differences in geometry are mainly ascribed to the size difference of the anions. The exceptionally high binding affinity toward fluoride anion can be explained by six-point hydrogen bonding resulting adaptation of geometry of the complex.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-421**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

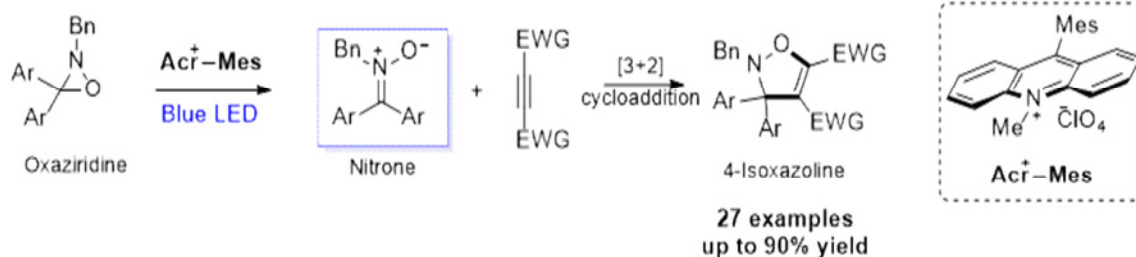
Efficient Synthesis of 4-Isoxazolines using Visible-Light Photoredox Catalysis

sangkook woo*, GwangSeok Jang¹

Department of Chemistry, University of Ulsan, Korea

¹*Chemistry, University of Ulsan, Korea*

4-Isoxazolines are an important class of heterocycles, widely present in many bioactive molecules. In addition to serving as drug and agrochemical targets, 4-isoxazolines are also valuable as synthetic building blocks in organic synthesis. Therefore, many methods have been developed for their synthesis. The photochemical reactions of organic compounds provide a concise way to form complex molecular skeletons. We report highly efficient synthetic method for 4-isoxazolines using visible light photoredox catalysis



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-422**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of asymmetric organic compounds for the use of new functional MOFs

Yuro Kim, Ho Hyeon Lee¹, Hakwon Kim^{2,*}, Hongil Jo³, Kang Min Ok³

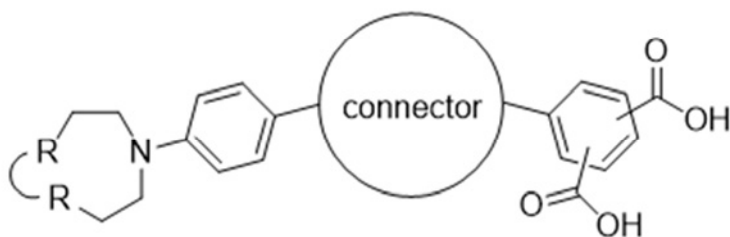
Department of Chemistry, Kyung Hee University, Korea

¹*Department of Medicinal Chemistry, Jungwon University, Korea*

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

³*Department of Chemistry, Chung-Ang University, Korea*

Metal-organic frameworks (MOFs) are compounds revealing extended structures consisting of metal ions and coordinated organic linkers. Depending on the coordination numbers and orientation of organic ligands, various dimensional backbones such as chains, layers, and three-dimensional frameworks are expected. In addition, many interesting material properties are observed by utilizing the functionality of the linkers and metal cations. In this work, we have designed and synthesized a series of novel dicarboxylic acids containing a variety of functional groups. The size, rigidity, and orientation of the newly synthesized organic linkers have been carefully controlled by varying the connectors using succinic acid or phthalic acid. The position of carboxylic acids has been also adjusted. Preliminary experiments on the synthesis of new MOFs by using the linkers are also presented.



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Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-423

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

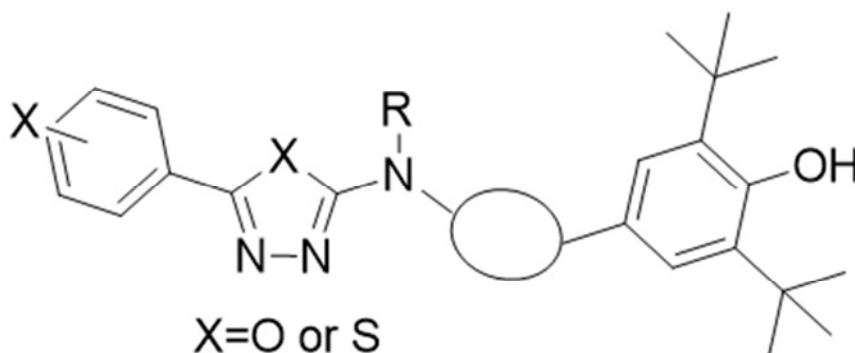
Synthesis and Antioxidant Activity of BHT Derivatives containing 2-Amino-1,3,4-Oxadiazoles or 2-Amino-1,3,4-Thiadiazoles

SooJin Park, TAEHOON LEE¹, Seowon Chang¹, Hakwon Kim^{1,*}

Department of Chemistry, Kyung Hee University, Korea

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

Butylated hydroxytoluene (BHT) is well known for antioxidant properties, because its phenolic –OH transforms to stable free radical due to the possibility of resonance stability of the resulting phenoxy radical. The combination of the known phenolic antioxidants, BHTs, with heterocyclic pharmacophores, such as 2-amino-1,3,4-oxadiazole or 2-amino-1,3,4-thiadiazole, in the same unit can be an interesting approach to discover novel more potent radical scavengers. In this study, a series of 5-aryl-2-amino-1,3,4-oxadiazole-BHT and 5-aryl-2-amino-1,3,4-thiadiazole-BHT derivatives was synthesized and screened for radical scavenging properties.



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Code: **ORGN.P-424**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

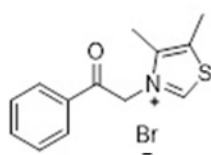
Synthesis of various 4,5-dimethylthiazolium salts and Potential Activity for AGEs Breaking

Inseok Ko, Hyunjin Lee¹, JiSue Lee¹, Hakwon Kim^{1,*}

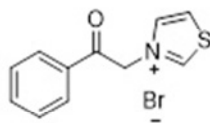
Department of Chemistry, Kyung Hee University, Korea

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

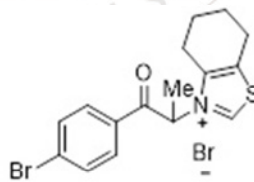
Advanced glycation end-products (AGEs) are proteins or lipids that become glycated as a result of exposure of sugars. They can be a factor in aging and in the development or worsening of many degenerative diseases, such as diabetes, atherosclerosis, chronic renal failure, and Alzheimer's diseases. Alagebrium and its derivatives were known as compounds that are thought to break some existing AGE crosslinks. In this work, we have synthesized various novel 4,5-dimethylthiazolium salts containing naphthalene or heterocyclic moieties and tested for AGE breaking.



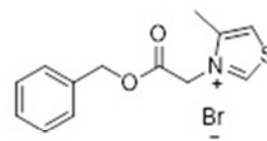
ALT-711
Alagebrium



PTB



C-16



C-36

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-425**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Antiviral Activities of Various Sterol Glycosides

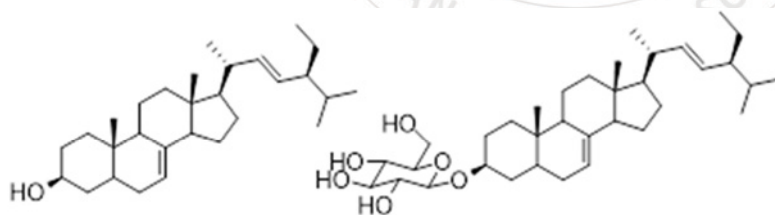
YOUNGKYOUNG CHO, Yeseul Park¹, Dowon Yoon², Hakwon Kim^{1,*}

Department of Chemistry, Kyung Hee University, Korea

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

²*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. Further biological investigation with spinasterol glycosides were needed, but due to the difficulty and inefficiency of isolation and synthesis of natural spinasterol and spinasterol glucose it has not been done. In the present study, we have synthesized natural spinasterol and spinasterol glycosides, and several new sterol glycosides from ergosterol, stellarsterol and ergostenol to test for the antiviral activity.



Spinasterol and Spinasterol glucose

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-426**

Area: Organic Chemistry

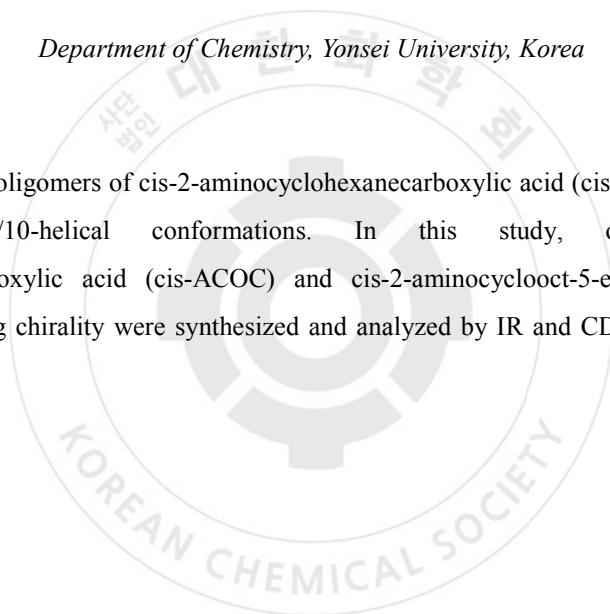
Type: Poster Presentation, Time: FRI 13:00~14:30

Characterization of β -peptides consisting of cyclic β -amino acids with an eight-membered ring constraint

MinKyung Kim, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

It has been shown that oligomers of cis-2-aminocyclohexanecarboxylic acid (cis-ACHC) with alternating chirality form 12/10-helical conformations. In this study, oligomers of cis-2-aminocyclooctanecarboxylic acid (cis-ACOC) and cis-2-aminocyclooct-5-enecarboxylic acid (cis-ACOE) with alternating chirality were synthesized and analyzed by IR and CD spectroscopic methods, respectively.



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Code: **ORGN.P-427**

Area: Organic Chemistry

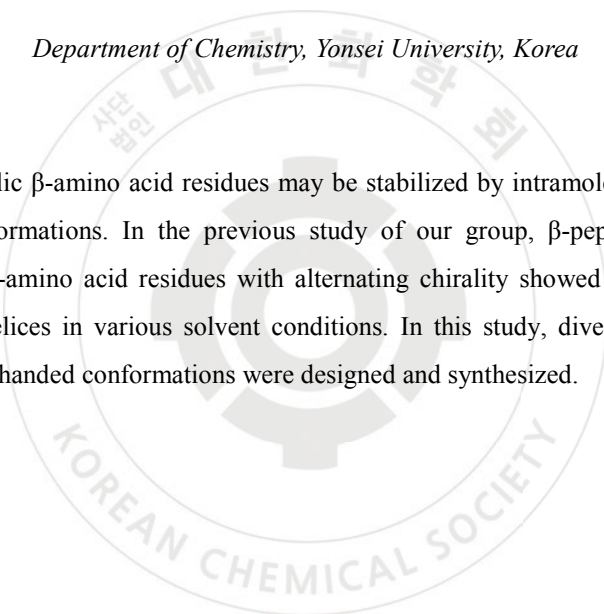
Type: Poster Presentation, Time: FRI 13:00~14:30

Characterization of β -Peptide Oligomers Containing cis-2-Aminocycloheptanecarboxylic Acid

Hoyang Son, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

Peptides containing cyclic β -amino acid residues may be stabilized by intramolecular hydrogen bonding to display helical conformations. In the previous study of our group, β -peptide hexamer of seven-membered-ring-based β -amino acid residues with alternating chirality showed different ratios between two opposite-handed helices in various solvent conditions. In this study, diverse control peptides that adopt only left- or right-handed conformations were designed and synthesized.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-428**

Area: Organic Chemistry

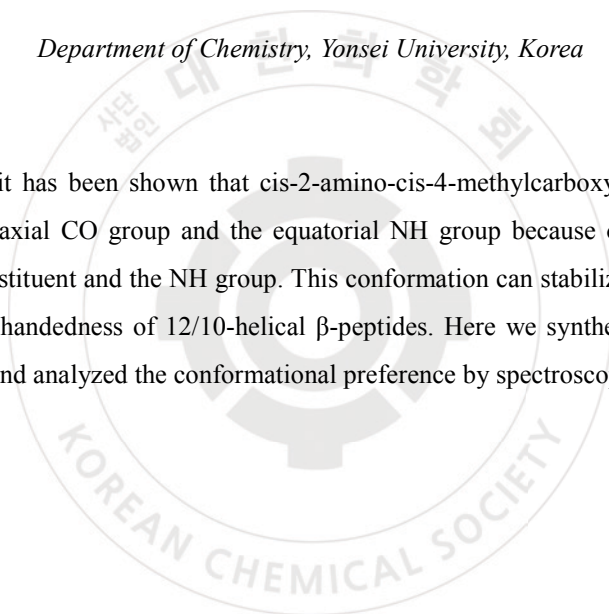
Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and conformational analysis of cis-2-amino-cis-5-methylcarboxylic acid

Sojung Kim, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

In the previous study, it has been shown that cis-2-amino-cis-4-methylcarboxylic acid adopted a local conformation with the axial CO group and the equatorial NH group because of 1,3-diaxial interaction between the methyl substituent and the NH group. This conformation can stabilize 11/9-helical folding of α/β -peptides or fix the handedness of 12/10-helical β -peptides. Here we synthesized cis-2-amino-cis-5-methylcarboxylic acid and analyzed the conformational preference by spectroscopic methods.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-429**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Chemo- and Stereoselective Crotylation of Aldehydes and Cyclic Aldimines with Allylic gem-Diboronate Ester

Jinyoung Park, SEOYOUNG CHOI, Seung Hwan Cho*

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

We report a highly chemo- and stereoselective crotylation of aldehydes and cyclic aldimines with allylic-gem-diboronate ester as a new type of organoboron reagent. The allylic-gem-diboronate ester undergoes the crotylation with aldehydes and cyclic aldimines in excellent stereoselectivity, forming anti-5,6-disubstituted oxaborinin-2-ols or (E)- δ -boryl-anti-homoallylic amines in high efficiency. The reaction shows a wide range of substrate scope and excellent functional group tolerance. The synthetic applications of the obtained products, including stereospecific C-C, C-O, and C-Cl bond formation, are also demonstrated

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-430

Area: Organic Chemistry

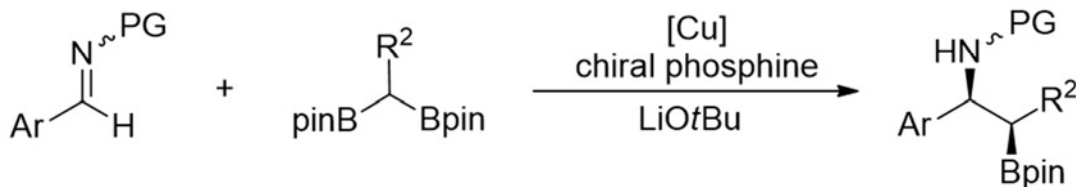
Type: Poster Presentation, Time: FRI 13:00~14:30

Copper(I)-Catalyzed Diastereo- and Enantioselective 1,2-Addition of 1,1-Bis[(pinacolato)boryl]alkanes to Imines: Synthesis of β -Aminoboronates

Jeongho Kim, Seung Hwan Cho*

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

The preparation of chiral β -aminoboron is important in synthetic chemistry because it constitutes a core structure in many biologically active compounds. Recently, several synthetic methods have been reported for the synthesis of chiral β -aminoboron including 1,2-aminoboration, hydroboration, ring opening and reductive amination reactions. In this poster presentation, we will describe an efficient copper(I)-catalytic system for diastereo- and enantioselective addition of 1,1-bis[(pinacolato)boryl]alkanes to protected imines to afford synthetically valuable chiral β -aminoboron compounds. The reaction exhibits a broad scope with protected imines and 1,1-bis[(pinacolato)boryl]alkanes, providing chiral β -aminoboronate esters in good yields with excellent diastereo- and enantioselectivity. The synthetic utility of the obtained β -aminoboronate esters will also be provided.



- Excellent diastereo- (up to >20:1) and enantioselectivity (up to 99% ee)
- Broad scope of imines and 1,1-bisborylalkanes
- Synthetic utilities

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-431**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

synthesis and analysis of energetic ionic salts

Kuktae Kwon^{*}, SeungHee Kim, So Jung Lee, Yeongjin Jeon¹

Agency for Defense Development, Korea

¹*University of Science & Technology, Korea*

Energetic materials are such compounds release high energy when they are decomposed. They are classified propellants, explosives and pyrotechnics. Energetic materials such as TNT, RDX have been studying for a long time. TNT was a major explosive during Worldwar-II and RDX was promising explosive for low cost and high performance. After age of RDX, very few explosives were developed and applied for the formulation of explosive. It means that it is very difficult to meet conditions which are physicochemical properties, cost, performance and sensitivity issues for next generation of high explosive. As an effort to develop new energetic materials, reaserch about high nitrogen content compound such as azoles was investigated in wide range, because of high heat of formation for N₂. Heat of formation is known to be closely related to the energetic properties. Also salt research area is opened for energetic materials, due to their extremely low vapor pressure and relatively high density. Here in, we report synthesis and analysis of triazolium salts for high energy materials.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-432**

Area: Organic Chemistry

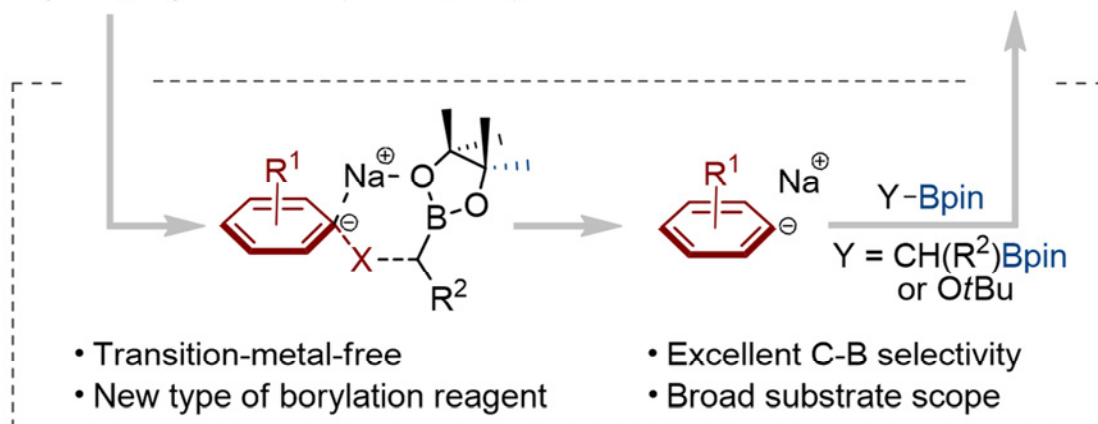
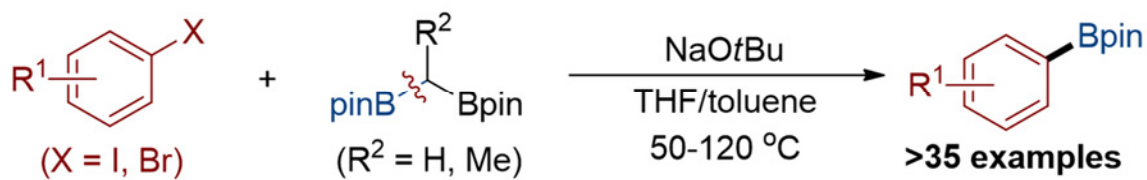
Type: Poster Presentation, Time: FRI 13:00~14:30

Chemoselective Coupling of 1,1-Bis[(pinacolato)boryl]alkanes for the Transition-Metal-Free Borylation of Aryl and Vinyl Halides: A Combined Experimental and Theoretical Investigation

Yeosan Lee, Jinyoung Park, Jeongho Kim, Seung Hwan Cho *

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

A new transition-metal-free borylation of aryl and vinyl halides using 1,1-bis[(pinacolato)boryl] alkanes as boron sources is described. In this transformation one of the boron groups from 1,1-bis[(pinacolato)boryl]alkanes is selectively transferred to aryl and vinyl halides in the presence of sodium *tert*-butoxide as the only activator to form organoboronate esters. Under the developed borylation conditions, a broad range of organohalides are borylated with excellent chemoselectivity and functional group compatibility, thus offering a rare example of a transition-metal-free borylation protocol. Experimental and theoretical studies have been performed to elucidate the reaction mechanism, revealing the unusual formation of Lewis acid/base adduct between organohalides and α -borylcarbanion, generated in situ from the reaction of 1,1-bis[(pinacolato)boryl]alkanes with an alkoxide base, to facilitate the borylation reactions.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-433**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Anion Binding Properties of meso-Imidazolyl Picket Calix[4]pyrroles

Hyouk Choi, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

Calix[4]pyrroles have been studied as versatile receptors for various anionic guests. Our long term interests for the development of the calixpyrrole-based receptors displaying higher affinity and selectivity toward carbonate anion prompted us to design and synthesis of new receptors that bears aromatic pickets on the diametrical meso-positions. Here, we report the synthesis and anion binding properties of new receptors bearing imidazolyl (or imidazolium) groups at diametrical meso-positions in cis-configuration. The synthesis was accomplished by acid-catalysed condensation of meso-imidazolyl-dipyrromethane with acetone, followed by isolation of the two isomers. The detailed anion binding studies of the synthesized receptors will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-434**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and properties of angled porphyrin trimer bearing non-aromatic porphyrin core

Hyebin Lee, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

meso-Alkylidenyl porphyrins are non-aromatic, conformationally flexible, tetrapyrrolic macrocycles that are joined to the porphyrin family most recently.^{1,2} The compounds exhibit few interesting physico-chemical properties such as unusual protonation selectivity, unique tautomerism and conformational irregularity. The compounds also display unusual protonation selectivity depending on the number of core N-Hs. As a part of our continuing efforts for the construction of the array of the porphyrins, we here report the synthesis and property of a porphyrin trimer bearing non-aromatic core. The synthesis has been accomplished by Sonogashira coupling of the corresponding A3B type-porphyrins and meso-alkylidenyl porphyrin. Detailed spectroscopic and prototropic properties will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-435**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and properties of anti-aromatic, hexapyrrolic expanded porphyrin analogues and their metal complexes

Yoorim Go, Dikhi Firmansyah, Chang Hee Lee*

Department of Chemistry, Kangwon National University, Korea

Calix[4]pyrroles have been studied as versatile receptors for various anionic guests. Our long term interests for the development of the calixpyrrole-based receptors displaying higher affinity and selectivity toward carbonate anion prompted us to design and synthesis of new receptors that bear aromatic pickets on the diametrical meso-positions. Judicious choice of meso-aryl groups could enable recognition of suitable anionic species through non-covalent forces such as anion- π interactions. For instance selective recognition and sensing of pyrophosphate and fluoride anions were achieved in cases of meso-pyridinium and meso-4-fluorophenyl calix[4]pyrroles respectively.^{1,2} Here, we report the synthesis and anion binding properties of new receptors bearing imidazolyl (or imidazolium) groups at diametrical meso-positions in cis-configuration. The synthesis was accomplished by acid-catalysed condensation of meso-imidazolyl-dipyrromethane with acetone, followed by isolation of the two isomers. The synthesized receptors were characterized by various spectroscopic techniques. The detailed anion binding studies of the synthesized receptors will be presented.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-436**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Aluminum Catalyzed Hydroboration of Carbonyl Compounds

Jaeun Ku, won kyu sin, Duk Keun An^{*}

Department of Chemistry, Kangwon National University, Korea

Reduction of carbonyl compounds to alcohols can be broadly classified into three categories, i) stoichiometric reduction with reducing agents, ii) metal-catalyzed hydrosilylations, and iii) metal-catalyzed and non-metal-catalyzed hydroborations. Among them, metal-catalyzed hydroboration of esters is known to be very limited. Here, we wish to report a new catalytic hydroboration of carbonyl compounds using aluminum reagents as catalyst. Recently, we investigated the catalytic hydroboration of carbonyl compounds including esters by treatment with pinacolborane and DIBALH(cat.) or LDBBA(cat.). This method is believed to be the first case of catalytic hydroboration using aluminum catalyst. Furthermore, we plan to study mechanism of this reaction through some kind of experiments.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-437**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

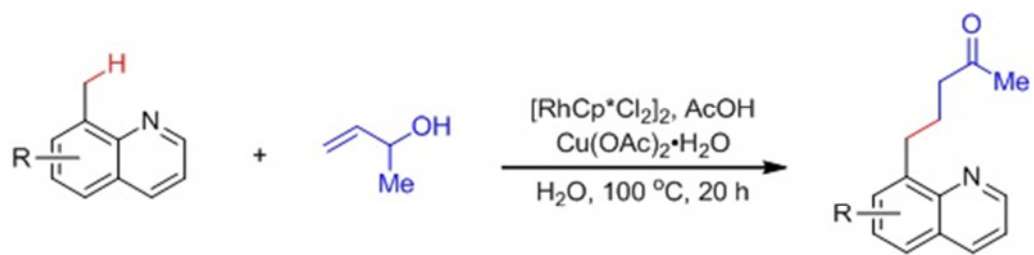
Cross-Coupling Reaction of 8-Methylquinolines with Allylic Alcohols Under Rhodium(III)-Catalysis

Saegun Kim, IN SU KIM^{1,*}

University of Pharmacy, Sungkyunkwan University, Korea

¹*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The rhodium(III)-catalyzed cross-coupling reaction of 8-methylquinolines with a range of allylic alcohols in water is described. This approach leads to the synthesis of various γ -quinolinyl carbonyl compounds, which are synthetically useful precursors for the construction of bioactive tetrahydroquinoline and azasteroid derivatives. Induced by the need to streamline the synthesis of valuable building blocks and complex molecules, the transition-metal catalyzed C–H bond activation has evolved as an important field in organic synthesis. It has attracted tremendous interest in developing cross-coupling reactions at low cost without the use of stoichiometric amounts of organometallic reagents. In particular, C(sp²)–H functionalization has been studied to a greater extent, whereas less research attention has been paid to the activation of C(sp³)–H bonds. In this area, sp³ C–H functionalizations have been executed with the assistance of a range of chelating auxiliaries such as amides, carboxylic acids, oximes, N-heterocycles, etc. In particular, 8-methylquinolines have been found to be good substrates for sp³ C–H functionalization due to their ability to form cyclometalated complexes. However, sp³ C–H alkylation of 8-methylquinolines has rarely been explored. Although the catalytic C–H bond functionalizations provide atom economy, which constitutes a great contribution to the cross-coupling reaction, most of these reactions have been carried out in organic solvents. In continuation of our Rh(III)-catalyzed sp² and sp³ C–H alkylations, we herein report for the first time the C(sp³)–H alkylation of 8-methylquinolines with allylic alcohols in water as a green solvent.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-438**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis and Analysis of Ring Strained Mild Energetic Plasticizer for PBX,

Yeongjin Jeon, Kuktae Kwon^{1,*}, SeungHee Kim¹, So Jung Lee¹

University of Science & Technology, Korea

¹*Agency for Defense Development, Korea*

PBX consist of explosives, binders, and plasticizers. Polymer binders provide dimensional stability and insensitivity to compound explosives. And Plasticizers give workability, insensitivity and physical properties when processing PBX and charging it into the body. Well known plasticizers are DOA (Dioctyl Adipate), DEHA(Bis (2-ethylhexyl) Adipate), DIBP (Diisobutyl Phtalate). These plasticizers are low in energy due to their simple structure. Therefore, there is a disadvantage that the performance is decreased by the content of the plasticizer. In an effort to improve this problem, many researchers on energizing plasticizers have tried a lot of research into introducing azide, nitrate, or nitro groups into the plasticizer using same method used in explosive. The performance of these energy plasticizers has certainly improved, but they are very sensitive and restriction on the PBX. In this study, Cyclobutane derivative as a basic structure was synthesized. The reason is to induce the energy increase by adding the ring stress to the plasticizer. And ring strained energetic group were introduced into both branches.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-439**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

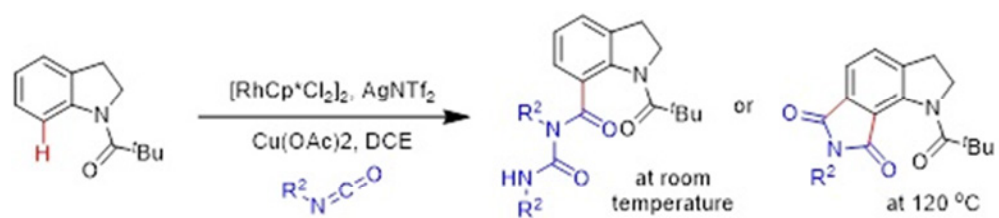
Synthesis and Cytotoxic Evaluation of N-Aroylureas Under Rh(III)-Catalyst via C-H Activation

Sukhun Lee, IN SU KIM^{1,*}

University of Pharmacy, Sungkyunkwan University, Korea

¹*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The rhodium(III)-catalyzed C-H amidation and subsequent C-N bond formation reaction of indolines with aryl and alkyl isocyanates at room temperature are reported. These transformations allow the generation of N-aroyleurea functionality at the C7-position of indolines, which is known as a crucial scaffold found in biologically active molecules. In addition, the synthesis of pyrroloindolidione derivatives is also described through sequential C6-amidation reaction and intramolecular cyclization of C7-amidated indolines. All synthesized products were evaluated for in vitro cytotoxic effect against human prostate adenocarcinoma cells (DU145), human breast cancer cells (MCF-7), and triple negative human breast cancer cells (MDAMB-231), respectively. Notably, compounds 4d and 4e with linear alkyl side chains were found to be highly cytotoxic, which is comparable to that of anticancer doxorubicin and cisplatin as positive controls. we herein present the unexpected formation of N-aroyleureas derived from indolines and aryl/alkyl isocyanates via the Rh(III)-catalyzed direct amidation reaction of indolines at the C7-position followed by subsequent C-N bond formation. In addition, all synthesized products have been evaluated for cytotoxic activity against various cancer cell lines such as human prostate adenocarcinoma cell lines (DU145), human breast cancer cell lines (MCF-7) and triple negative human breast cancer cell lines (MDA-MB-231), and were found to display promising cytotoxic effect competitive with well-known anticancer doxorubicin and cisplatin.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-440

Area: Organic Chemistry

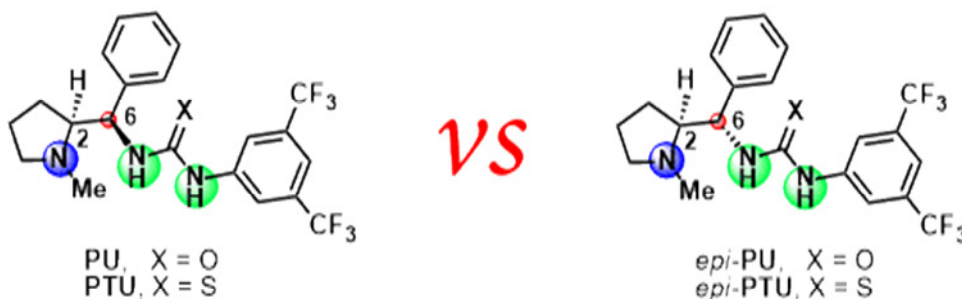
Type: Poster Presentation, Time: FRI 13:00~14:30

The Important Role of the Newly Formed Stereocenter on the Catalytic Activity of Proline Derived Bifunctional Organocatalysts

HUI JIN, Cho Soo Min, JUYEOL LEE, do hyun ryu *

Department of Chemistry, Sungkyunkwan University, China

As one of the most important classes of non-covalent organocatalysts, tertiary amine-(thio)urea organocatalysts have proven quite successful in accomplishing various asymmetric organic transformations. Recently, we reported a series of novel L-proline-derived tertiary amine bifunctional organocatalysts (PTU and PU), which were applied to asymmetric Michael additions to nitroolefins using dithiomalonates¹ and 2-oxochroman-3-carboxylate esters² as nucleophiles. In order to better understand the effects of the relative stereochemistry at C2/C6 on the catalytic activity, the C6 epimeric catalysts epi-PTU and epi-PU were newly synthesized and their catalytic performances were compared with PTU and PU in various Michael reactions of nitrostyrene in terms of reactivities and stereoselectivities.³ The experimental results indicate that a proper relative stereochemistry at C2 and C6 in L-proline-derived bifunctional organocatalysts is important for successful catalysis, and that catalysts (PTU and PU) with the 2S,6R configuration are much more efficient.



Better chiral scaffold for the bifunctional catalysis

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-441**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis, Structure, and Electrochemical Properties of Quinoxaline-Annulated Tetrathiafulvalene Pyrroles

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¹*Department of Chemistry, Sookmyung Women's University, Korea*

Conjugated donor-acceptor systems have been attracted due to their diverse applications such as artificial photosynthetic, solar cell, and nonlinear optical materials. Among a variety of the electron donating moieties, tetrathiafulvalene (TTF) derivatives are well-known key constituents for donor-acceptor systems. Especially, pyrrole-fused TTF derivatives are used as important building blocks because they can be readily converted to a variety of supramolecular functional materials.^[1] On the other hand, quinoxaline, a nitrogen containing bicyclic compound, is widely employed as a versatile electron-deficient building block including dyes, pharmaceuticals, antibiotics and various functional electronic materials.^[2]

With such consideration in mind, here we firstly present the synthesis of a series of quinoxaline-annulated TTF pyrrole derivatives as well as bis-quinoxaline-TTF. These molecular structures have been fully characterized by ¹H and ¹³C-NMR, High Resolution-Mass spectra, and X-ray crystallography. Their electrochemical and photophysical properties are examined by UV-Vis, fluorescence spectroscopy, cyclic voltammetry and EPR spectroscopy. In common, all these derivatives exhibit intramolecular charge transfer (ICT) band. Upon the addition of either Brønsted–Lowry acid or Lewis acid, largely red-shifted ICT band were observed.

[1] J. S. Park, J. Kim, Y.-H. Kim, J. L. Sessler, *RSC Adv.*, 2015, **5**, 69259-69262

[2] J. J. Bergkamp, S. Decurtins, S.-X. Liu, *Chem. Soc. Rev.*, 2015, **44**, 863-874

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-442

Area: Organic Chemistry

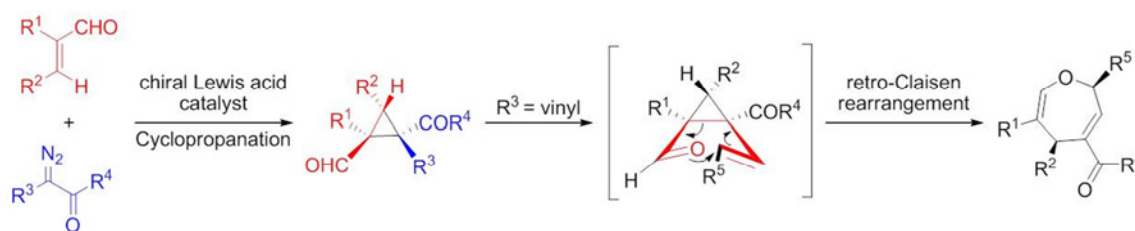
Type: Poster Presentation, Time: FRI 13:00~14:30

COBI-catalyzed enantioselective synthesis of cyclopropane and its retro-Claisen rearrangement to 2,5-dihydrooxepine

Su Yong Shim, Cho Soo Min, do hyun ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Over the past decades, considerable attention has been devoted to the development of asymmetric methodologies for the synthesis of cyclopropane derivatives. However, the examples of enantioselective cyclopropanation reactions via Michael-Initiated Ring Closure (MIRC) between α,β -unsaturated aldehyde and diazo compounds are uncommon. Recently, we developed chiral oxazaborolidinium ion (COBI) catalyzed enantioselective cyclopropanation of α - or α,β -substituted acroleins with various α -alkyl diazo compounds providing highly functionalized cyclopropane compounds with excellent trans/cis ratio (>20:1) and stereoselectivity (up to >99% ee). The synthetic utility of this methodology was demonstrated in the first total synthesis and absolute structure determination of Hamavellone B exhibiting antimalarial activity. We envisaged that this approach could be extended to enantioselective synthesis of 2,5-dihydrooxepine. While 2,5-dihydrooxepine has been synthesized by retro-Claisen rearrangement of the corresponding vinylcyclopropylcarboxaldehyde, examples of asymmetric synthesis of 2,5-dihydrooxepines using this approach are rare due to the multiple steps required for the preparation of the chiral vinylcyclopropylcarboxaldehyde. Here, we report COBI-catalyzed enantioselective synthesis of 2,5-dihydrooxepine through tandem-cyclopropanation-retro-Claisen rearrangement with α -vinyl diazo compounds. A wide range of 2,5-dihydrooxepines with aliphatic and aromatic group were obtained in high yield (up to 86%) and excellent enantioselectivity (up to >99% ee).



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-443**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Asymmetric Formation of β -Hydroxysilane Using Diazoalkane Compounds and Various Aldehydes

Jae-Yeon Kim, do hyun ryu *

Department of Chemistry, Sungkyunkwan University, Korea

Organosilanes are useful building blocks for organic synthesis because they are good substrates for many regio- and stereoselective reactions to construct carbon-carbon and carbon-heteroatom bonds in high stereoselectivities. Despite a growing focus toward synthetic efforts, access to chiral organosilanes in a highly enantioenriched form remains a great challenge and the development of new methods continues to be an active area of research. In this research, we synthesized highly enantioselective β -hydroxysilane reduced from α -silyl ketone catalyzed by chiral boron catalyst. The synthetic utility of this method was demonstrated by the synthesis of allylic silanes which are very versatile synthetic reagents for the regioselective introduction of the allyl group into electrophiles.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-444**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

D-D- π -A structures metal free dyes planarity effect in thin film dye sensitized solar cells

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Department of Chemistry, Sungkyunkwan University, Korea

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Structural planarity is the most crucial parts of effecting intramolecular charge transfer (ICT). We designed and produced metal free dyes and to control planarity we introduced carbazol, indoline and quinoline units. The planar structure shows high molar absorptivity, caused by fast ICT. Similarly, the power conversion efficiency (PCE) of planar dye exhibits higher values. Therefore, indoline based RK-3 dyes, D-D- π -A structure, shows 10.3% of PCE when the active thickness is 3.5 μm .

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ORGN.P-445

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

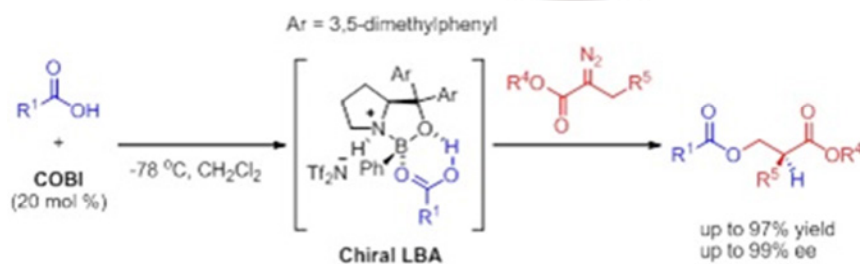
Enantioselective Protonation-Nucleophilic addition of α -Benzyl Diazoesters with Chiral Oxazaborolidinium Ion-Activated Carboxylic Acids

Ki-Tae Kang, Seungtae Kim, Geum-Sook Hwang^{1,*}, do hyun ryu^{*}

Department of Chemistry, Sungkyunkwan University, Korea

¹*Korea Basic Science Institute, Korea*

The asymmetric protonation-nucleophilic addition is an ideal synthetic strategy for preparing optically pure α or β -acyloxy carbonyls and α or β -hydroxy carboxylic acid derivatives, which are valuable building blocks for the construction of natural products and other biological active molecules. In this presentation, chiral proton donor which is prepared with chiral oxazaborolidinium ion (COBI) catalyst and carboxylic acid will be discussed. This chiral proton donor is highly effective reagent for asymmetric protonation-nucleophilic addition. The reaction proceeded in good yields (up to 97%) with excellent enantioselectivities (up to 99% ee).



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-446**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

In Situ Generation of Sulfur (II) Ylides from Thiolates and their Structural Studies

Jun Ki Kim^{*}, Yeong-Joon Kim¹, Hwan Jung Lim², Seong Jun Park^{2,*}

Center for Medicinal Chemistry, Chungnam National University / Center for Medicinal Chemistry, Korea

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

²*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology (KRICT), Korea*

Since it has not been reported the sulfur (II) ylide in community, we aim to explore the preparation of the stable sulfur (II) ylide. Due to difficulties for the direct confirmation of the carbene ion of sulfur (II) ylide, our initial effort focused on the indirect approach using the reported thiophene synthesis. We believe that the desired thiophene could be obtained after the formation of the sulfur (II) ylides. By changing the substituent groups in N,S-acetals, we investigated how structural effects could influence stability and reactivity of sulfur (II) ylides.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ORGN.P-447**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Transition-Metal-Free Regioselective Alkylation of Pyridine N-Oxide Using 1,1-Diborylalkanes as Alkylating Reagents

Chiwon Hwang, Woohyun Jo, junghoon Kim, Seung Hwan Cho*

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

In this presentation, an unprecedented base-promoted deborylative alkylation of pyridine N-oxides using 1,1-diborylalkanes as alkyl sources is introduced. The reaction proceeds efficiently for a wide range of pyridine N-oxides and 1,1-diborylalkanes with excellent regioselectivity. The utility of the developed method is demonstrated by the sequential C-H arylation and methylation of pyridine N-oxides. The reaction also can be applied for the direct introduction of a methyl group to 9-O-methylquinine N-oxide, thus it can serve as a powerful method for late-stage functionalization.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ORGN.P-448**

Area: Organic Chemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

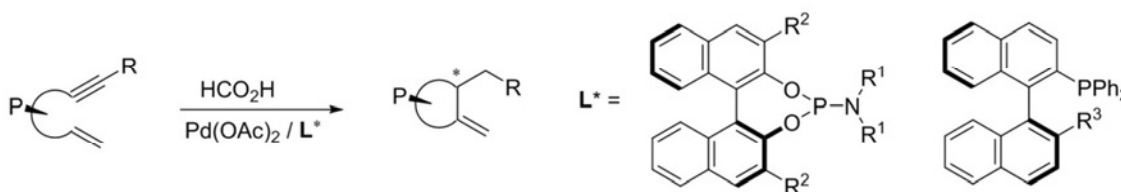
Expansion of Substrate Scope in Asymmetric Cycloreduction of α,ω -Enynes by Chiral Palladium-Catalysts Coordinated with Monodentate Phosphorus Ligands

Hee Gun Park, Seung Hwan An¹, Jin Wook Han^{1,*}, Chang Ho Oh^{1,*}

Department of Chemistry, Hanyang University, 한양대학교 나노과학 기술 연구소, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Recently we achieved both high catalytic activities and high enantioselectivity in asymmetric cycloreduction of 1,6-enyne by palladium catalysts coordinated with chiral monodentate phosphorus ligand, especially phosphoramidites, in the presence of formic acid, which gave optically active cyclized organic compounds from N-tethered α,ω -enynes. Herein, we wish to report that the substrate scope has been expanded to various α,ω -enynes tethered by carbon or heteroatoms. We found that catalytic activities and enantioselectivities varied according to the substrate types.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-294**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design, Synthesis, and Enzyme Inhibitory Activity of Novel Aminopyrimidinylisoindolines against FAK and ACK1

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Department of Chemistry, Korea University, Korea

¹*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

Focal adhesion kinase (FAK) is a non-receptor tyrosine kinase that transduces signaling from a diverse group of stimuli to control a variety of cellular pathways and processes, including cell proliferation, migration, morphology, and cell survival. FAK is overexpressed in many tumors, including those derived from the head and neck, colon, breast, prostate, liver, and thyroid. 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, FAK and ACK1 have been proposed as potential targets in cancer therapy and small molecule inhibitors for use as potential cancer therapies have been developed. The purpose of this study is to develop the potent compounds as dual kinase inhibitors against FAK and ACK1. Based on the structural features of PF-562,271 and ASP-3026 as FAK and ACK1 inhibitors, a series of aminopyrimidinylisoindoline derivatives were designed and synthesized. The enzymatic assay against FAK and ACK1 and cell-based assay against five cancer cell lines for the synthesized compounds were carried out.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-295**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and biological evaluation of a novel [¹⁸F]DMFB as a potential PET agent for malignant melanoma

Ayoung Pyo, Dong Yeon Kim*

Department of Nuclear Medicine, Chonnam National University Hwasun Hospital, Korea

The incidence of malignant melanoma has been increasing worldwide and there is still no effective treatment. Because of this cancer is a very aggressive, early detection in the earliest stages is very important to improve the survival of patients. In this study, we synthesized novel ¹⁸F labeled benzamide derivative. Furthermore, we evaluated biological characteristics in B16F10 (mouse melanoma) tumor bearing mice and lung / lymph node metastatic models. [¹⁸F]SFB was synthesized and used as prosthetic group. Amine derivative was dissolved in DMSO and added to dried [¹⁸F]SFB. The mixture was heated at 60°C for 30 min and purified by using HPLC. The microPET images were obtained at 10, 30, and 60 min after *i.v.* injection of [¹⁸F]DMFB (7.4MBq) in B16F10 bearing nude mice. The static images at 10, 30, and 60 min were acquired for 10 min. The overall non decay-corrected radiochemical yield was approximately 10–15%. In biodistribution studies, tumor uptake of [¹⁸F]DMFB (10, 30, 60 and 120 min % ID/g: 9.24, 10.8, 13.0, 10.6) retained from 10 to 120 min. Liver uptake of [¹⁸F]DMFB (10, 30, 60 and 120 min % ID/g: 11.19, 5.76, 2.47, 0.45) decreased from 10 to 120 min and showed fast clearance from liver. We performed microPET studies with [¹⁸F]DMFB. B16F10 tumor and metastasis lesions were visible after *i.v.* injection and [¹⁸F]DMFB retained for whole time (over 60 min). [¹⁸F]DMFB demonstrated malignant melanoma with high tumor uptake and specifically targeted metastatic lesions in B16F10 lung / lymph node metastasis model. [¹⁸F]DMFB might have a potential to be utilized as a novel melanoma imaging agent for PET.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-296**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Theoretical investigation on oxidation potential analysis of tamoxifen derivatives

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Institute for Basic Science, Korea

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

Tamoxifen, (Z)-2-[4-(1,2-diphenyl-1-butenyl)phenoxy-N,N-dimethylethanamine] , breast cancer drug, interrupts that estrogen molecule binds to estrogen receptor and inactivates estrogen receptor. Tamoxifen itself is the prodrug but it turns out to endoxifen after metabolism in liver. When Tamoxifen becomes endoxifen (N-desmethyl-4-hydroxytamoxifen), the binding activity with estrogen receptor increased as much as 30 – 100 times. Therefore the Oxidation activity of tamoxifen to endoxifen can be understood by oxidation potential between two species. From the various experiments, it is observed that metallocene tag decreases the oxidation potential of tamoxifen oxidation process. [1] Herein we theoretically investigated about the oxidation process of metallocene tag-attached tamoxifene derivatives, ferrocifen and cymantrene. By introducing ion-pairing model to this system, we could successfully describe experimental value and it has meaningful itself that how does ion-pair works with target molecule in the low dielectric media. After then we analyzed the electron density of oxidative species and figure out that which location is the most effective to control the oxidation potential of tamoxifene derivatives. From these studies, we could understand how does the metallocene tag decreases the oxidation potential and suggest potential candidates. Also we completed the reaction mechanism of tamoxifen under base condition, and conclude that which condition makes oxidation easier and drives to new-stable compound. [2][1] K. Wu, S. Top, E. A. Hillard, G. Haouen, W. E. Geiger, Chem. Commun. 2011, 47, 10109-10111.[2] J. Y. Park, H. Nam, Y. Lee, W. E. Geiger, M.-H. Baik, manuscript in preparation (2017).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-297**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design and Synthesis of the Novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

JIWOONG LIM, Seokkyu Kim¹, Dong Hoi KIM², Jae Wook Lee³, SANG MIN LIM⁴, Jae Yeol Lee^{1,*}, Ae Nim Pae^{3,*}

KHU-KIST Department of Converging Science and Tech, Kyung Hee University, Korea

¹Department of Chemistry, Kyung Hee University, Korea

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SHIP2, a lipid phosphatase that hydrolyzes PI(3,4,5)P₃ to PI(3,4)P₂, plays a pivotal role in regulating several intracellular signaling pathways and is involved in the pathogenesis of various diseases through its phosphatase activity and localization changes. Recent studies have suggested that inhibition of SHIP2 could produce a significant benefits in the treatment of Alzheimer's Disease (AD). AD is characterized by amyloid- β (A β) plaques in the brain and neurofibrillary tangles of hyper-phosphorylated tau, a microtubule-binding protein. The Fc γ RIIb-SHIP2 signaling axis could provide the missing link between A β and tau pathologies. Notably, A β ₁₋₄₂ induces Fc γ RIIb phosphorylation to recruit SHIP2, followed by increased production of PI(3,4)P₂, disrupting the balance of phosphoinositide metabolism leading to tau hyperphosphorylation and memory impairment in neurons. Therefore, inhibition of SHIP2 can be an effective therapeutic strategy in AD. For developing SHIP2 inhibitors, we performed the phosphatase assay with malachite green using in house libraries. From high-throughput screening, we found hit compounds, and synthesized new derivatives based on the hit scaffolds. Among the synthesized compounds, DTC0461 was identified as a potent SHIP2 inhibitor. The optimization of novel SHIP2 inhibitors to further enhance potency and physicochemical properties is now in progress. We have presented the first example of a small molecule SHIP2 inhibitors for AD. This compound will help to elucidate physiological functions of SHIP2 and its involvement in AD.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-298**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and anti-melanogenic activities of the chalcone derivatives

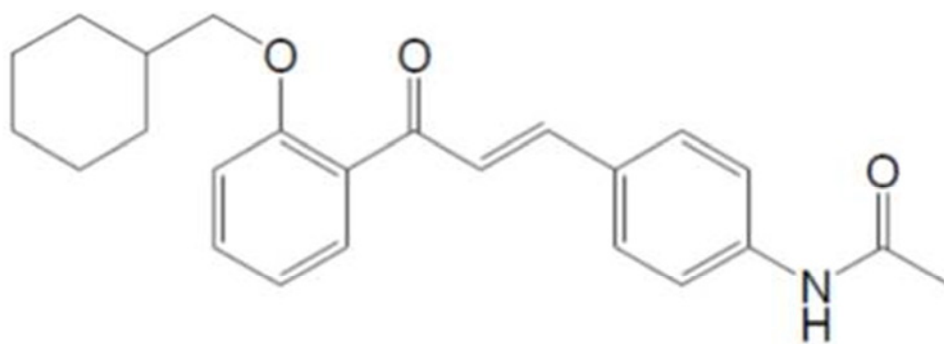
Jung Youl Park^{*}, Jong-Min Han¹, Byung-Hak Kim²

Dept. of Applied Chemistry, Daejeon University, Korea

¹*Department of Life Science, Daejeon University, Korea*

²*Department of Pharmacology, Seoul National University, Korea*

Melanin is a group of natural pigments and is the major factor responsible for skin and hair color in mammals. It has several beneficial functions, including skin protection from harmful ultraviolet (UV) radiation and prevention of cancer development. However, abnormal accumulation and hyperpigmentation of melanin result in pigmentation disorders such as freckles, melasma, chloasma, ephelides, senile lentiginos and melanoderma and can induce inflammation such as eczema, allergic contact dermatitis, and irritant contact dermatitis, which can lead to serious and emotionally distressing problems. We previously demonstrated that the chalcone derivative 1-(2-cyclohexylmethoxy-6-hydroxyphenyl)-3-(4-hydroxymethyl-phenyl)-propenone (chalcone-21) exhibited anti-melanogenic activity in B16F10 melanoma cells. To increase its anti-melanogenic activity, we synthesized 21-kinds of novel compounds as its derivative and determined their inhibition effects of melanin production in a-MSH-induced B16F10 cells. Among them, chalcone-21-21 exhibited the strongest inhibition of cellular melanin production with an IC₅₀ value of 0.54 mM, compared with 4.9, 38.5 and 148.4 mM of IC₅₀ values of chalcone 21, kojic acid and arbutin, respectively. As the molecular mechanisms, we identified chalcone 21-21 suppressed the expression and transcriptional activity of tyrosinase, the rate-limiting enzyme of melanogenesis, as well as its enzyme activity. Chalcone 21-21 suppressed also the expression of TRP-1, TRP-2, and MITF. In addition, chalcone 21-21 suppressed not only phosphorylation of CREB and ERK1/2, but also the transcriptional activity of MITF and CRE. Our results demonstrated chalcone-21-21 is an effective anti-melanogenic agent and may benefit the treatment of hyperpigmentation disorders.



Chalcone-21-21 (C₂₄H₂₇NO₃)



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-299**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of 6-hydroxy-4-oxo-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinoline-5-carboxylic acid derivatives as Potential Inhibitor of *S. pneumoniae* serotypes

Srigouri Huddar, Chul Min Park¹, Sunkyung Lee^{1,*}

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

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

Studies from USA, Europe and Asia reported that antibiotic resistance rates from 18% to 84% observed, were associated with the emergence of multidrug resistance in *S. pneumoniae* and will continue to make currently available antibiotics essentially ineffective. Discovery of new therapies for treating drug resistant pneumococcal infections is therefore, urgently needed. A series of 6-hydroxy-4-oxo-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinoline-5-carboxylic acid derivatives were prepared and evaluated for their inhibitory activities on three different types of *Streptococcus pneumoniae* serotypes; *S. pneumoniae* serotypes ATCC 49617TM (19F, wild type), ATCC BAA-1663TM (15B, drug resistant), and ATCC 700904TM (19A, erythromycin resistant). From this studies, we identified potent compounds on resistant strains as well as wild type. Reference 1. Identification of Antipneumococcal Molecules Effective Against Different *Streptococcus pneumoniae* Serotypes Using a Resazurin-Based High-throughput screen, *Assay and Drug Development Technologies*, 2017, 15(5), 198-209.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-300**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

On-resin Cyclic Peptide Synthesis via Cysteine side chain anchoring Pyroacm resin

KangTae Kim, Young Dae Gong^{*}, Vinayak Juvekar

Department of Chemistry, Dongguk University, Korea

Cyclic peptides are regarded as important synthetic compounds because of their various biological activity. The constraint imposed from cyclization leads to enhancing biological activity as well as increasing resistance to proteolysis compared with linear peptides. Various lengths of cyclic peptides are synthesized to improve well-known cyclization method's weakness using Pyroacm linker. The process involves initial immobilization of cysteine into pyroacm resin under acidic condition to avoid racemization. The β -elimination during peptide elongation controlled by using bulky protecting group at C-terminal. After elongation of peptide of required size, various on-resin cyclization processes have been screened. Peptides of smaller length showed both cyclization and homodimerization whereas peptide of six to seven amino acid residue, homodimerization was minimal. The process has been utilized to synthesis various cyclic peptide library containing four to seven amino acid residues.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-301**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of 1-Alkyl- 2-amido-Benzo[*d*]imidazoles on Solid-phase via Desulfurative Cyclization of Thiourea Resin

HYUNJEONG YOO, seung ju yang, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

In this study, we synthesized 1-Alkyl- 2-amido-Benzo[*d*]imidazoles derivatives. Substituted *N*¹-alkylbenzene-1,2-diamines reacted with polymer supported isothiocyanate resin derived from 4-benzyloxy-2-methoxybenzylamine (BOMBA) resin through a reaction with carbon disulfide, trimethylamine and *p*-TsCl in tetrahydrofuran to generate thiourea intermediate resin. The desulfurative cyclization of thiourea intermediate resin was successfully conducted with using 2-chloro-1,3-dimethylimidazolium chloride (DMC) and *N,N*-diisopropylethylamine in dichloromethane (DCM) to afford 2-amino-Benzo[*d*]imidazoles resin, and then diverse acid chlorides were introduced at 2-amine position. In case of 3-nitrobenzoyl chloride, nitro group was reduced by Tin(II) chloride in DMF followed by reaction with amino acids and aldehydes for further diversification. Finally, we obtained various 1-Alkyl- 2-amido-Benzo[*d*]imidazoles by cleavage of the corresponding resin under trifluoroacetic acid (TFA) in dichloromethane (DCM).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-302**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Combinatorial synthesis of Drug-like Pyrrolopyrimidine analogues with a High level of diversity in solution-phase

Si Yeon Han, eunsil Lee¹, Young Dae Gong^{*}

Department of Chemistry, Dongguk University, Korea

¹*Medicinal Chemistry Laboratory, Dongguk University, Korea*

Pyrimidine based derivatives are known to have a broad spectrum of biological activities such as anti-cancer, antimicrobial, anti-inflammatory, antiviral activity. Furthermore, many researchers have conducted study about biological activity of pyrimidine scaffold since success of Gleevec(Imatinib). Recently, pyrrolopyrimidine is also identified as a potent MRP1 inhibitors which mediated Multidrug resistance and JAK3(Janus kinases 3) inhibitors. In this context, as a part of our on-going project aimed at a construction of small molecule library, we have tried to synthesize pyrrolopyrimidines equipped with diverse functional groups in combinatorial way. As a result, we've obtained numerous pyrrolopyrimidine derivatives in high yields and purities. References 1. Sven Marcel Schmitt, Katja Stefan, Michael Wiese. *Biochimica et Biophysica Acta* 1859 (2017) 69–79 .2. Michael P. Clark, Kelly M. George, Roger G. Bookland, Jack Chen, Steven K. Laughlin, Kumar D. Thakur, Wenlin Lee, Jan R. Davis, Ed J. Cabrera, Todd A. Brugel, John C. VanRens, Matthew J. Laufersweiler, Jennifer A. Maier, Mark P. Sabat, Adam Golebiowski, Vijay Easwaran, Mark E. Webster, Biswanath Dea and George Zhanga. *Bioorganic & Medicinal Chemistry Letters* 17 (2007) 1250–1253

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-303**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Solid-Phase Parallel Synthesis of a 1,3,4-Oxadiazole Based β -Turn Mimetic Library

AIZHAN ABDILDINOVA, seung ju yang, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

β -turn is a protein secondary structure element and known to be modulating protein-protein interactions. 1,3,4-oxadiazole derivatives also known to have a wide range of biological activities such as anticancer, antibacterial, antimicrobial, anti-inflammatory, etc. Combination of a small molecule fragment with peptide motif can improve pharmacokinetic properties of both peptide and small molecule and provide more effective drug probes. In this study, we developed an efficient and mild method for the synthesis of α -amino acid substituted 1,3,4-oxadiazoles that mimic the bioactive β -turn structural motif of proteins. Initial synthesis starts from the reaction between thiosemicarbazide resin with α -amino acid and further cyclization to the 1,3,4-oxadiazole. Further functionalization with adding more α -amino acids for the chain prolongation and cleavage from the supporting resin can provide library of desired β -turn mimetic compounds.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-304**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design, Synthesis of *N*-(5-methyl-2-(phenylamino)thiazolo[5,4-d]pyrimidin-7-yl)benzenesulfonamide derivatives as an inhibitor of cyclin-dependent kinases(CDKs)

HYEJIN KWON, eunsil Lee¹, Young Dae Gong*

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Roscovotine, also called Seliciclib, is biologically well used inhibitor which is targeting cyclin-dependent kinases(CDKs). CDKs(CDK1, CDK2, CDK5 and CDK7), drug targets of Roscovitine, are involved in cell cycle including mRNA process, transcription and the cellular differentiation. Roscovitine regulates abnormal cell cycle by binding to ATP binding site. Therefore, it is currently evaluated as a potential drug of cancers, neurodegenerative diseases, inflammation, viral infections, polycystic kidney disease etc. In this context, we've tried to design a new drug targeting CDKs by referring to the structure of Roscovitine. We've synthesized Thiazolopyrimidine-based compound By replacing the imidazole which is part of purine, the main structure of Roscovitine, with thiazole. Also, various substituents were introduced at carbons(2,6,8) of thiazolopyrimidine to increase the structural diversity. Starting from 4,6-dichloro-2-methylpyrimidin-5-amine, we have synthesized about 100 kinds of compound by substituting 8 kinds of benzenesulfonamide at carbon 6 in thiazolopyrimidine which were synthesized by cyclization of 4,6-dichloro-2-*N*-pyrimidin-5-amine using 20 kinds of isothiocyanate.

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Synthesis of biological active *N*-(3-phenyl-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-yl)benzenesulfonamide derivatives

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Vast majority of marketed drugs introduce contains hetero cyclic core skeleton. Among these heterocycles, triazolopyrimidine is a representative hetero cyclic structural motif since its derivatives have been shown diverse biological activity and pharmaceutical interests. Thus, triazolopyrimidine has been targeted to synthesize by many organic chemists and medicinal chemists and there are several reported methods to afford this core skeleton in the literature. In this context, we have tried to synthesize diverse triazolopyrimidine analogues in combinatorial way equipped with sulfonamide and aryl group at 6 and 9 positions, respectively. As a result, we've obtained numerous triazolopyrimidine derivatives in good yield.

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A Highly Efficient Diversification of 1,3,4-Oxadiazole and 1,3,4-Thiadiazole analogues on Solid-phase

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In this work, we constructed 1,3,4-oxadiazole and 1,3,4-thiadiazole library with high level of skeletal diversity on solid-phase organic synthesis. The 1,3,4-oxadiazole and 1,3,4-thiadiazole core skeleton resin was successively afforded through desulfurative cyclization of thiosemicarbazide resin derived from a reaction between isothiocyanate resin and various hydrazides. To functionalize 1,3,4-oxadiazole and 1,3,4-thiadiazole resin, we used various alkyl halides, acid chlorides, isocyanates, isothiocyanates, aldehydes, boronic acids and amino acids. Finally, these functionalized 1,3,4-oxadiazole and 1,3,4-thiadiazole resins were treated with trifluoroacetic acid in dichloromethane, affording diverse 1,3,4-oxadiazole and 1,3,4-thiadiazole analogues in good yields and high purities.

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Area: Medicinal Chemistry

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Synthesis of azetidine-3-carboxylic acid derivatives as novel S1P₁ agonists

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Multiple sclerosis (MS) is an autoimmune disorder affecting central nervous system (CNS) in which the insulating covers of nerve cells in the brain and spinal cord are damaged, resulting in disrupting the ability of parts of the nervous system to communicate. Sphingosine-1-phosphate (S1P) is a bioactive sphingolipid that regulates a diverse range of physiological processes such as lymphocyte trafficking, cardiac function, vascular development, and inflammation. S1P receptors (S1PRs) are a class of G protein-coupled receptors, which are divided into five subtypes: S1P₁, S1P₂, S1P₃, S1P₄, and S1P₅. Fingolimod (FTY720) as a S1P₁ agonist was approved as the first oral drug for reducing relapse rate in multiple sclerosis. However, it also activates S1P₃, S1P₄ and S1P₅ and causes various side effects such as bradycardia. Thus, we have focused on discovery of selective and potent S1P₁ agonists. We designed and synthesized the compounds including azetidine-3-carboxylic acid and various biphenyl moiety. Synthesized compounds were biologically evaluated against S1P₁. The results of in vitro assay and structure-activity relationship (SAR) will be presented in detail.

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Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and biological evaluation of new pyrimidine derivatives for kinase inhibitor

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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, SIK kinase has three types of SIK1, SIK2, and SIK3. SIK2 kinase (salt-inducible kinase 2) is a serine / threonine protein kinase belonging to the AMP-activating protein kinase (AMPK) family and is overexpressed in 30% of ovarian cancer patients. Prostate cancer is generally a cancer that can be treated surgically, but about 10-15% of patients have difficulty with surgery and require medication. SIK2 kinase may be a target for cancer treatment. It is also reported to be involved in triple-negative breast cancer (TNBC), a difficult breast cancer to treat. SIK2 receptor kinase has been shown to occur at very high frequency in ovarian, prostate, and breast cancer cells, and has recently been suggested as a new target for kinase inhibitors. Therefore, inhibition of SIK2 can be an effective therapeutic strategy in these cancers. For developing SIK2 inhibitors, we synthesized new pyrimidine derivatives based on the hit scaffolds. Among the synthesized compounds, KIST301613 was identified as a lead SIK2 inhibitor. The optimization of novel SIK2 inhibitors to further enhance potency and physicochemical properties is now in progress.

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Dendritic Polymer based Multi-Photosensitizers for Enhanced Photodynamic Therapy

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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. That is the reason why we combined dendritic polymer with photosensitizers to get enhanced photodynamic effect.

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Design and synthesis of indazole derivatives as DYRK1B inhibitors

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Dual-specificity tyrosine phosphorylation-regulated kinase 1B (DYRK1B) is over-expressed in several different tumor types such as colon, ovarian, and pancreatic cancer. Recent studies have demonstrated inhibition of DYRK1B could be an attractive target for cancer therapy. In this study, we designed and synthesized indazole derivatives as novel DYRK1B inhibitor that ultimately can be developed as an anticancer drug. These derivatives exhibited potent inhibitory activity toward DYRK1B in an in vitro assay. Structure modification of indazole derivatives revealed structure-activity relationships for DYRK1B inhibition and enabled to design very potent DYRK1B inhibitors. We will measure the cytotoxicity by the CCK assay, the physical properties, and pharmacokinetic.

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Type: Poster Presentation, Time: THU 11:00~12:30

Novel dual inhibitors of amyloid beta and tau aggregation for treatment of Alzheimer's Disease

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Alzheimer's disease(AD) is a chronic neurodegenerative disease that is the most common form of dementia. It is still unclear what AD causes, but AD features 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 targeting compounds, such as amyloid aggregation inhibitors, β -secretase inhibitors and so on, have been failed to cure AD patients. Therefore, our rationale of dual inhibitors is to reduce the generation of NFT as well as AP that may relate to causes of AD. We obtained hit compound(DTC0100) which inhibits tau aggregation in Bi-FC assay. Then, we optimized to improve the efficacy of tau aggregation inhibition and pharmacokinetic properties. The synthesized DTC0359 showed excellent inhibition of tau aggregation ($IC_{50} = 0.4 \mu M$) and was also lower amyloid- β aggregation ($IC_{50} = 1.0 \mu M$) in vitro as dual inhibitors. Furthermore, DTC0359 significantly decreases both A β aggregation in ex-vivo (APP/PS19 mice) and Tau aggregation in ex-vivo (Tau-P301L-BiFC mice). Optimization of pharmacokinetic properties and in vivo study is ongoing.

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Two Photon Probes of Prostate-Specific Membrane Antigen (PSMA) for the Imaging of Colon Cancers

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Prostate-specific membrane antigen (PSMA) is an accessible cell-surface bound homodimeric endopeptidase, which can be efficiently targeted using urea-based derivatives of glutamic acids such as 2-[3-(1,3-dicarboxypropyl)ureido]pentanedioic acid (DUPA). PSMA is usually absent in normal adult tissues, exception made for normal prostate tissue and duodenum. The tumor-targeting imaging of various PSMA ligands has been validated in rodents and in cancer patients, using nuclear medicine or molecular fluorescence procedures. Here we will present the design of two photon probes with a PSMA binding motif, and their application for the diagnosis of colon cancer in patients.

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Benzenesulfonyl Amide Derivatives as Selective mPGES-1 Inhibitors Ameliorate the Cognitive Impairment in Animal Model

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A novel series of phenylsulfonyl hydrazide derivatives reduced LPS-induced PGE₂ levels in RAW 264.7 macrophage cells via an inhibition of mPGES-1 enzyme. However, two regioisomers of phenylsulfonyl hydrazide exhibiting a wide range of biological activities were formed depending on the reaction conditions. In order to avoid this synthetic problem, new benzenesulfonyl amide (5: MPO-0112) as an analogue of potent phenylsulfonyl hydrazide (MPO-0063) was synthesized and biologically evaluated in vitro. As a result, MPO-0112 strongly suppressed LPS-induced PGE₂ production (IC₅₀: 0.34 μM) with excellent selectivity over COX-enzymes (COX-1 and 2) and also inhibited mPGES-1 enzyme (IC₅₀: 7.37 μM) comparable to those of MPO-0063. According to the recent studies on the close correlation between up-regulation of mPGES-1 and Alzheimer's disease, we investigated whether MPO-0112 can ameliorate scopolamine-induced memory impairment using the passive avoidance test. The memory impairment-ameliorating effect of MPO-0112 (1.0 mg/kg, p.o.) was effective comparable to that of donepezil (5 mg/kg, p.o.) as a positive control. In addition, MPO-0112 exhibited a favorable in vitro CYP profile, which is suggestive of no potential drug–drug interactions. Therefore, these overall results suggest that MPO-0112 as selective mPGES-1 inhibitor may be a novel therapeutic agent for diseases associated with cognitive deficits, such as Alzheimer's disease.

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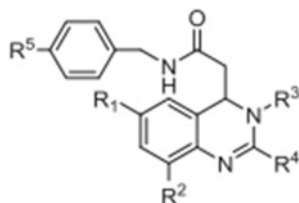
Anticancer and Analgesic Activities of Fluoro-substituted 3,4-Dihydroquinazoline Derivatives

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As a bioisosteric strategy to overcome the poor metabolic stability of lead compound KYS05090S, a series of new fluoro-substituted 3,4-dihydroquinazoline derivatives was prepared and evaluated for T-type calcium channel (Ca_v3.2) block, cytotoxic effects and liver microsomal stability. Among them, compound 8h (KCP10068F) containing 4-fluorobenzyl amide and 4-cyclohexylphenyl ring potently blocked Ca_v3.2 currents (>90% inhibition) at 10 μM concentration and exhibited cytotoxic effect (IC₅₀ = 5.9 μM) in A549 non-small cell lung cancer cells that was comparable to KYS05090S. Furthermore, 8h showed approximately a 2-fold increase in liver metabolic stability in rat and human species compared to KYS05090S. Based on these overall results, 8h (KCP10068F) may therefore represent a good backup compound for KYS05090S for further biological investigations as novel cytotoxic agent. In addition, compound 8g (KCP10067F) was found to partially protect from inflammatory pain via a blockade of Ca_v3.2 channels.



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Synthesis and Synergistic Effect of T-type Calcium Channel Blockers as a Anticancer Agents on Human Lung Cancer

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We synthesized new 3,4-dihydroquinazoline derivative containing ureido group, KCP10043F and evaluated for T-type calcium channel inhibitory activity, cytotoxicity, and cell cycle arrest against human lung cancer (A549) cells. KCP10043F showed both weaker T-type Ca²⁺ channel inhibitory activity and less cytotoxicity against A549 cells than parent compound KYS05090S [4-(benzylcarbamoylmethyl)-3-(4-biphenyl)-2-(*N,N,N'*-trimethyl-1,5-pentanediamino)-3,4-dihydroquinazoline 2 hydrochloride], but it exhibited more potent G₁-phase arrest than KYS05090S in A549 cells. This was found to be accompanied by the downregulations of cyclin-dependent kinase (CDK) 2, CDK4, CDK6, cyclin D2, cyclin D3, and cyclin E at the protein levels. However, p27^{KIP1} as a CDK inhibitor was gradually upregulated at the protein levels and increased recruitment to CDK2, CDK4 and CDK6 after KCP10043F treatment. Based on the strong G₁-phase cell cycle arrest of KCP10043F in A549 cells, the combination of KCP10043F with etoposide (or cisplatin) resulted in a synergistic cell death (combination index = 0.2–0.8) via the induction of apoptosis compared with either agent alone. Taken together with these overall results and the favorable *in vitro* ADME (absorption, distribution, metabolism, and excretion) profiles of KCP10043F, therefore, it could be used as a potential agent for the combination therapy on human lung cancer.

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Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Biological Evaluation of Phenylsulfonyl Hydrazide Derivatives as Novel mPGES-1 Inhibitors

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A novel series of phenylsulfonyl hydrazide derivatives, which were derived from the high throughput screening hit compound 1 ($IC_{50} = 5700$ nM against PGE_2 production), for a potent inhibitor of mPGES-1 is described. Compound 8n turned out to be most potent lead compound with IC_{50} value of 4.5 nM and 6.9 nM, respectively, against LPS-1 induced PGE_2 and NO production in RAW 264.6 macrophage cells. In addition, 8n was about 30- and > 150-fold more potent against mPGES-1 enzyme in a cell-free assay ($IC_{50} = 70$ nM) than MK-886 and hit compound 1, respectively. Molecular docking suggests that compound 8n could inhibit PGE_2 production by blocking the PGH_2 binding site of human mPGES-1 enzyme.

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Cationic Chlorin and Polyoxometalate Nanocarrier Synthesized by Click Chemistry for Nuclear Targeting and Highly Efficient Photodynamic Therapy In Vitro

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Simple click chemistry enabled the synthesis of neutral clicked chlorin, which was converted to cationic clicked chlorin that formed a clicked chlorin-polyoxometalate (POM) supramolecular complex as a nanocarrier via electrostatic interactions between the cationic clicked chlorin and the polyanionic POM. The cellular uptakes of clicked chlorin, cationic clicked chlorin, and the cationic clicked chlorin-POM complex against A549 cell lines were confirmed by confocal laser scanning microscopy. Clicked chlorin, cationic clicked chlorin, and the cationic clicked chlorin-POM complex were accumulated in cytoplasm as well as nuclei. Cell viability results showed that the cationic clicked chlorin-POM complex (IC₅₀, 338.8 nM) and free cationic clicked chlorin (IC₅₀, 342.4 nM) exhibited significantly enhanced, more than 10 times higher, photocytotoxicity compared to clicked chlorin (neutral, IC₅₀, 3.81 μM) based on better nuclear targeting. This results suggest that this cationic clicked chlorin-POM complex is a highly promising photosensitizer for PDT without aggregation and dark cytotoxicity for no side effect.

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Synthesis of biphenyl-3-ylmethylamine derivatives as 5-HT₇ receptor modulators

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5-HT₇ receptor is the most recently discovered serotonin receptor that localized within CNS such as thalamus, hypothalamus, limbic and cortical regions. Recent reports suggest that 5-HT₇ receptor is involved in the regulation of body temperature, circadian rhythms, learning and memory, as well as neuronal excitability, inflammatory processes and smooth muscle relaxation of cerebral arteries. 5-HT₇ receptor knockout animal studies have provided demonstrative proofs that 5-HT₇ receptor is considered as a potential target for treating depression, sleep disorder, and neuropathic pain. There has been much attention to discover 5-HT₇ modulators to obtain therapeutic benefits. We have designed and synthesized compounds including biphenyl-3-ylmethylamines. Using Suzuki reaction and reductive amination, total 12 final compounds with biphenyl moiety were synthesized and biologically evaluated against 5-HT₇ receptor. Among them, two compounds showed the best binding affinities with K_i values of 9.3 and 6.8 nM, respectively. The results of binding affinity assay and structure-activity relationship (SAR) to 5-HT₇ receptors will be presented in detail.

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Synthesis of Bombesin Tethered to ^{18}F Labeled Mesoporous Silica Nanoparticles as a PET Tracer for Image Guided Surgery and Therapy

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Positron Emission tomography (PET) 영상의 높은 투과도를 이용하여 image guided surgery 를 할 경우 비 침습적으로 암의 위치를 정확히 파악할 수 있다는 장점이 있다. PET 을 image guided surgery 에 더 잘 적용 시키기 위해서 암에 선택적으로 결합하고 PET 에 적합한 방사성원소가 표지된 probe 의 개발이 필요하다. 열 안정성과 생체 적합성이 좋은 Mesoporous silica nanoparticle (MSN)에 GPCR 유도체에 잘 결합한다고 알려진 Bombesin peptide 를 연결한 형태를 기반으로 하여 image guided surgery 에 유용한 새로운 PET probe 를 합성하였다.

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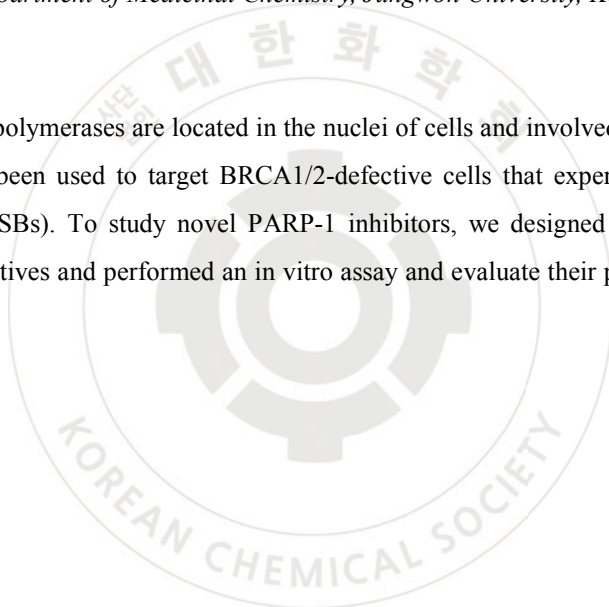
Type: Poster Presentation, Time: THU 11:00~12:30

Novel Benzamide Derivatives as Potent PARP-1 Inhibitors

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The poly(ADP-ribose) polymerases are located in the nuclei of cells and involved in DNA damage repair. PARP inhibitors have been used to target BRCA1/2-defective cells that experience increases in DNA single-strand breaks (SSBs). To study novel PARP-1 inhibitors, we designed and synthesized several novel benzamide derivatives and performed an in vitro assay and evaluate their potential as possible anti-cancer therapeutics.



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Discovery of Cholesteryl Ester Transfer Protein Inhibitor for the Treatment of Dyslipidemia/Cardiovascular Diseases

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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 CE 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 is about anacetrapib from Merck in clinical phase III, waiting for the final results. Recently, we designed a novel series of small molecules as CETP inhibitor for ASCVD and over 130 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 (vehicle, anacetrapib 10 mpk QD, DN201929 10 mpk QD, and DN201929 30 mpk QD) 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.

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Synthesis of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

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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.

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EGFR Allosteric Inhibitors for Lung Cancer

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Erlotinib (Tarceva) & Gefitinib (Iressa) are currently in clinic use as epidermal growth factor receptor (EGFR) kinase inhibitors for non-small-cell lung cancer (NSCLC). However, their clinical efficacy is limited by both their mechanism-based toxicity and the development of drug-resistance mutations, including the gatekeeper T790M mutation. Afatinib, a quinazoline-based irreversible pan-EGFR inhibitor dubbed as second generation EGFR TKI, is limited in wide clinical use due to unwanted adverse effect such as severe rash and diarrhea. Osimertinib is a pyrimidine-based irreversible third generation EGFR-TKI and features selective EGFR T790M inhibition while sparing wild-type EGFR activity. However, during osimertinib clinical study, various acquired resistances were reported. In particular, polar nucleophilic cysteine mutation into polar non-nucleophilic serine at EGFR 797 position was detected in resistant patients. To address newly identified EGFR T790M/C797S mutants, new strategic approach is attempted. Unlike conventional catalytic site inhibitors, allosteric site inhibitors may provide novel inhibitors for EGFR T790M/C797S mutants and bring different mutational profiles for combination therapy with current EGFR-TKIs. In this presentation, strategy for EGFR allosteric inhibitors and current research progress will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-324**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Discovery of Novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

Seo Yoon Choi, Ae Nim Pae^{1,*}, Kyu-Sung Jeong^{*}, JIWOONG LIM², Jae Wook Lee¹, Dong Hoi KIM¹, SANG MIN LIM³

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Alzheimer's disease (AD) is characterized by the progressive loss of memory and the neuronal degeneration. The pathological hallmarks of AD are the presence of senile plaques consisting of A β peptide and neurofibrillary tangles (NFT) formed by abnormally hyperphosphorylated tau. Recent studies showed that the src homology 2 (SH2) containing inositol 5-phosphatase 2 (SHIP2) is a key mediator in delivering the toxic signal of A β to tau by binding to the phosphorylated Fc γ RIIb. Also, reducing the activity or amount of SHIP2 in mice that present the symptoms of Alzheimer's disease reduced the hyperphosphorylation of the tau protein in their neurons and restored their memory to normal levels. Here, we synthesized a series of novel SHIP2 inhibitors based on hit compounds from high-throughput screening and their inhibitory effects were verified in malachite green phosphate assay. Among them, DTC0310 exhibited potent inhibition effect. However, it was not favorable in terms of its pharmacokinetic profiles. To improve the activity and cell permeability, further modifications of the compound was examined. In the process of modification for better pharmacokinetic properties, DTC0441 showed favorable inhibition effect. With this promising assay result, measuring the drug-like properties of DTC0441 is on process. This compound may provide crucial insight into a SHIP2 inhibitor, which could be utilized as a therapeutic tool for the treatment of AD.

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Code: **MEDI.P-325**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of Novel Anti-Hepatitis C Virus Agent Targeting NS5A

Yoojin Jeong, Soon Bang Kang¹, Jeong Tae Lee², GYO CHANG KEUM^{3,*}

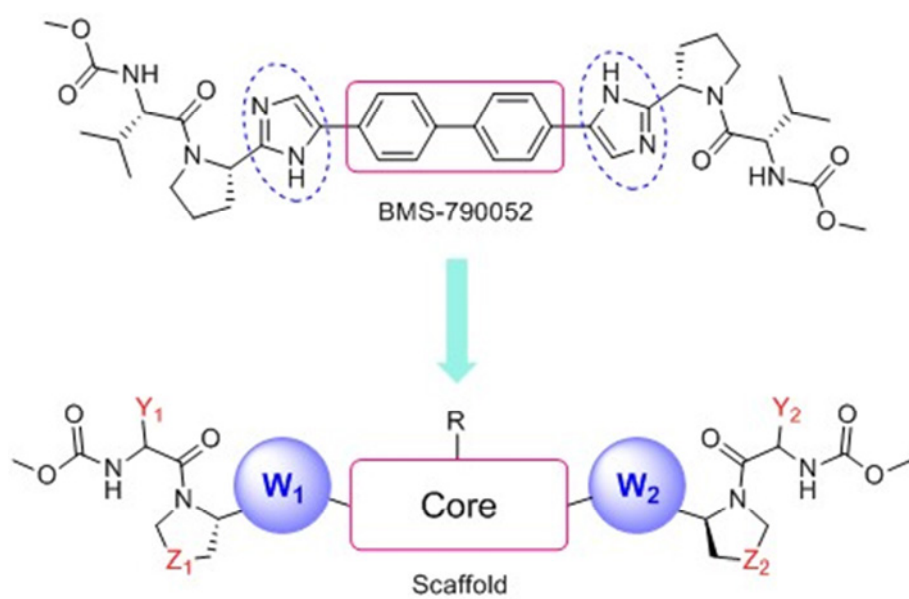
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Hepatitis C virus (HCV) is a leading cause of acute and chronic liver disease. About 180 million people are infected with HCV, which can lead to liver cirrhosis, hepatocellular carcinoma and consequently death. In addition to NS5B and NS3/4A protease inhibitor, NS5A was proved to be a promising target for the treatment of HCV. Several NS5A inhibitors such as BMS-790052 were launched recently and some were under clinical trials. We prepared a series of NS5A inhibitors possessing new scaffold and evaluated their activities against HCV cell lines. Among them, several compounds showed potent anti-HCV activity. Herein, we present anti-HCV activity of the hit compounds against various HCV genotypes and resistant strains mutated at L31V, Y93H of NS5A.



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Code: **MEDI.P-326**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Biological Activity of Tetrahydroisoxazolopyridine as S1P₁ Receptor Agonist

Young Jin Choi, Ji Soo Seo¹, SEON HEE SEO², Ghilsoo Nam^{3,*}

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²*Center for Neuromedicine, Korea Institute of Science and Technology, Korea*

³*Korea Institute of Science and Technology, Korea*

Multiple Sclerosis (MS) is an inflammatory and chronic disease of the CNS. MS is a demyelinating disease in which the insulating covers of nerve cells in the brain and spinal cord are damaged. This damage disrupts the ability of parts of the nervous system to communicate. In 2010, Novartis developed the first oral drug Fingolimod as a S1P receptor agonist. Fingolimod binds S1P₁ receptor and effects as a functional antagonist. Initially, the ligand binds S1P receptor-1 (S1P₁R) and then leads to internalization of S1P₁R on T-cells. Down-regulation of S1P₁R on lymph node T-cells renders lymphocytes unresponsive to the egressive signal and therefore prevents infiltration of pathogenic T-cells into the CNS. However, Fingolimod is a non-selective S1P₁R and then induces several side effects such as bradycardia (when Fingolimod binds S1P₃R). In this study, we tried to design new structures for compounds selectively bind to S1P₁R and S1P₃R agonist on the basis of the structure of BAF-312. In this poster, synthesis and biological activity tetrahydroisoxazolopyridine compounds as S1P₁ receptor agonist are described.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

QSAR Predictability Comparison between Deep Neural Network and Traditional Machine Learning Methods

Yongil Seo, Young Ju Seo, YongJoon Jang, JA YEON MOON, Namseok Kim, Ky-Youb Nam^{*}, Sinyoung Kim¹, Kwang-Hwi Cho¹, Jeong Hyeok YOON²

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In recent years, artificial neural network (ANN) model have been improved and the development of hardware has attracted the interest to deep neural network (DNN) and it has been applied in various fields example for automatic speech recognition, image recognition and customer relationship management. In particular, various machine learning techniques such as support vector machine (SVM) and multiple linear regression (MLR) as well as neural networks have been used in the field of quantitative structure-activity relationship (QSAR) for predicting the activities of compounds. In this study, we performed DNN methods to predict the toxicity of compounds by building some predicting models of hERG inhibitors which has an important toxicity on the discovery of drugs. In addition, we compared predictability between the DNN and the machine learning techniques such as SVM, MLR and ANN that have been previously developed. In the quantitative models, the MLR and ANN methods were compared with the DNN method. In the qualitative model, the SVM and Random forest methods were compared the DNN method.

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Code: **MEDI.P-328**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

IinQ attenuates systemic inflammatory responses via selectively impairing the Myddosome complex formation upon TLR4 ligation

Yunkyoung Hwang, Young Goo Kang, Byunghoon Ahn¹, Hee Nam Lim², ILL YOUNG LEE^{2,*}

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A selective, small-molecule inhibitor of the TLR4 signaling complex upstream of the IKK would likely provide therapeutic benefit for NF- κ B-mediated inflammatory disease. Brazilin was identified as a selective upstream IKK inhibitor targeting the Myddosome complex. In this study, using a cell-based ubiquitination assay for IRAK1 and a chemical library comprising of brazilin analogues, a novel small molecule, 2-hydroxy-5,6-dihydroisoindolo[1,2-a]isoquinoline-3,8-dione (IinQ) with the tetracyclic skeleton of the brazilin, was identified as a selective and potent inhibitor of IRAK1-dependent NF- κ B activation upon TLR4 ligation. In RAW264.7 macrophages, IinQ drastically suppressed activation of upstream IKK signaling events including membrane-bound IRAK1 ubiquitination and IKK phosphorylation by the TLR4 ligand, resulting in reduced expression of proinflammatory mediators including IL-6, TNF- α , and nitric oxide. Interestingly, IinQ did not suppress NF- κ B activation via the TLR3 ligand, DNA damaging agents, or a protein kinase C activator, indicating IinQ is specific for TLR4 signaling. Analysis of upstream signaling events further confirmed that IinQ disrupts the MyD88-IRAK1-TRAF6 complex formation induced by LPS treatment, without affecting TLR4 oligomerization

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Code: **MEDI.P-329**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Predicting acute oral toxicity of chemicals by QSAR approach

JaeYong Lee, Byeong Hun Lee, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

Oral toxicity is the toxicity of drugs that enter the digestive tract due to ingestion or absorption, impairing the function of the organism and altering organs or tissue. Approximately 2,000 chemical substances enter the world market each year, and more than 300 kinds of chemicals enter the market every year in Korea. Therefore, a toxicity tests are required to evaluate the toxicity of the compound to prevent adverse effects on human health or the environment. Unfortunately, toxicity test are time and cost consuming, and poses an ethical problem. The use of in silico method based on computer tools to solve these problems is fast and cost-effective to test chemical toxicity as an ethical alternative. The approach to achieving this goal successfully is the quantitative structure-activity relationship(QSAR), which use the mathematical expression of chemical structure information. In this study, LD50 data according to OECD Guideline 401 were collected from eChemPortal website to predict QSAR model. The molecular descriptors was calculated from 2D chemical structures using the PreADMET program. The data set is divided into training set(60%) used in the model development process and external test set(40%) used in the model validation process. 2D chemical descriptors and machine learning methods such as multiple linear regression(MLR) and support vector machine(SVM) were used to develop predictive QSAR model. The chance correlation and model predictability was verified by y-scrambling method and external validation. Also reliable prediction range is set in the kNN-based applicability domain.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Computational studies of the structure-activity relationships of small molecular inhibitors for EGFR and androgen receptor

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¹*Dept. of Chemistry and Biochemistry, UCLA, United States*

Detailed understanding of the drug-target interaction profiles can accelerate the drug discovery process by providing guiding principles for the rational drug design. We utilize advanced molecular dynamics MD simulation techniques to quantify the binding affinity profiles and the inhibitor induced conformational changes of EGFR kinase and androgen receptor (AR). We rationalized how clinically implicated mutations of EGFR kinase modulate the potency profiles of selective inhibitors the kinase. Molecular dynamics (MD) simulations showed that the mutations influence both the conformational equilibrium and the binding affinity to the target conformation of the kinase that the inhibitors recognize. Computed binding affinity changes were in quantitative agreement with the experimental potency profiles. In addition, we studied how the binding of the inhibitors influence the conformational characteristics of the androgen receptor (AR). Previously, it was envisioned that the binding of the AR ligands induces conformational changes in the ligand binding domain, that is correlated with the activity of the ligand. The binding of enzalutamide, a selective inhibitor of AR, alters the orientation of the helix 12. On the other hand, the binding of dihydrotestosterone (DHT) did not influence the structural integrity of the ligand binding domain. Based on the computational results, we proposed a structure-activity relationship (SAR) model that explains the efficacy of the AR inhibitors.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of QSAR models for predicting subchronic inhalation toxicity

Do Hyung Kim, Byeong Hun Lee, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

Subchronic inhalation toxicity is toxicological information obtained from long-term repeated exposure by the inhalation route. This toxicity data provides information on the hazards of chemicals during inhalation in the long term. However, there is currently no long-term inhalation toxicity information registered for a lot of chemicals. Because this test is complex experiments and it takes a long time and requires a lot of money. One solution to this problem is QSAR(Quantitative Structure-Activity Relationship). QSAR studies that satisfy regulatory requirements can provide useful tools for predicting long-term toxicity of untested chemicals. The aim of this study was to develop a Quantitative Structure-Activity Relationship (QSAR) model to predict sub-chronic toxicity inhalation. Subchronic inhalation toxicity data (rats, 13weeks, 5-7 days, 6hours) according to OECD test guideline 413 were obtained from echemportal website. Molecular descriptors and chemical fingerprint were calculated from 2D molecular structure using PreADMET and KNIME program. Data sets were divided into training set(60%) and test set(40%) based on structure diversity by RDKit fingerprint. 2D descriptors, fingerprint and machine learning methods such as multiple linear regression(MLR) and support vector machine(SVM) were used to develop predictive QSAR model. The chance correlation and predictability of these method were validated by y-scrambling method and external validation. The reliable prediction range of model is set in the kNN-based applicability domain(AD).

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Code: **MEDI.P-332**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Chemically induced target degradation of anaplastic lymphoma kinase (ALK) by Target Degraducers (TDs)

Dong-Ho Lee, Jae du ha¹, Duck-Hyung Lee, Jong Yeon Hwang^{2,*}

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Recently, a new and powerful technology called "proteomosis targeting chimeras" (PROTAC) has been actively applied in the field of drug development. Treatment of PROTAC molecule, which contains a ligand for the targeted protein, a ligand for E3 ubiquitin ligase binding, and a linker for connection of two ligands, successfully induced targeted protein degradation, thereby inhibiting cancer growth in in vivo animal model study. Anaplastic lymphoma kinase (ALK) gene fused to various partner genes are observed in 3–7% of non-small cell lung cancer (NSCLC) in humans. The constitutively activated ALK fusions play an essential role in cancer growth and survival. In this study we aimed to discover novel ALK target degraders (TDs) by applying PROTAC technology. LDK-378 (ceritinib) as an ALK ligand and VHL or CRBN as an E3 ubiquitin ligase were used. Hydroxyproline analogs (HP-7) and pomalidomide were used for VHL and CRBN E3 ligase ligands, respectively. All TDs synthesized in this study were evaluated in enzymatic- and cell-based assays. ALK degradation by TDs were confirmed by western blotting in SU-DHL-1 cell lines. In vivo antitumor activities were evaluated in xenograft mouse model with H3122 cell lines.

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Code: **MEDI.P-333**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

4-Phenylamino-1H-pyrazolo[3,4-d]pyrimidin-4-yl-acrylamide derivatives as novel irreversible Bruton's tyrosine kinase inhibitors and their biological activities

DukWoon Kim, Hyeon Seok jung, Jong Yeon Hwang¹, PILHO KIM¹, jae du ha², do hyun ryu, Sung Yun Cho^{2,*}

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Bruton's tyrosine kinase (BTK), a non-receptor tyrosine kinase, plays major roles in the B cell receptor signal transduction pathways regulating activation, survival, proliferation, and differentiation of B-lineage lymphoid cells. Mutations in gene encoding human BTK lead to X-linked agammaglobulinemia (XLA) in humans and X-linked immunodeficiency (Xid) in mice. Dysregulation of BTK signaling pathway is implicated with the pathogenesis of B cell lymphoma because B cells play a central role in the pathogenesis of several autoimmune diseases and B cell malignancies. Indeed, there have been tremendous number of clinical trials for either monotherapy or combined with other possible treatment, and inhibition of BTK has been considered as an effective and attractive therapeutic target for B cell related malignancies. In this report, we synthesized a series of novel 4-phenylamino-1H-pyrazolo[3,4-d]pyrimidin-4-yl-acrylamide derivatives that were substituted with phenyl moieties and evaluated BTK kinase inhibitory activity and cell based proliferation assay. Some of the compounds displayed excellent activity in vitro enzyme and cell-based assay.

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Code: **MEDI.P-334**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Discovery of Transglutaminase 2 Inhibitors for Renal Cell Carcinoma (RCC)

JiHee Kang, Ga young Park¹, Minsoo Song^{*}

Daegu Gyeongbuk Medical Innovation Foundation, Korea

¹*DGMIF, Korea*

Transglutaminase 2 (TGase 2, E.C. 2.1.2.13) is an enzyme that catalyzes an isopeptide bond between protein glutamine and lysine residues, resulting in a covalent crosslink. In renal cell carcinoma (RCC) cell lines, TGase 2 is highly overexpressed compared to normal cell lines and which deplete p53 into aggregates in autophagosome, leading to p53 depletion by the process of autophagy. This instability of p53 by TGase 2 regulation can cause tumor cells to avoid cell death and consequently have tumor cells grow. As such, the development of a new inhibitor of TGase 2 could be an effective strategy to treat RCC. In order to develop TGase 2 inhibitors, we have designed new type of scaffold of small molecule inhibitors for RCC. Over 250 compounds were synthesized and their biological activity were tested by in vitro enzyme assay and cell-based assay. Series of compounds were selected for ADME/T test and xenograft experiments. Among the tested compounds, we have identified that a lead compound DN201782 showed promising inhibitory efficacy both in vitro and in vivo against TGase 2. Herein, experimental data and xenograft results are presented in detail.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthetic chloride transporters promote apoptotic cell death by disrupting cellular ion homeostasis

Seong-Hyun Park, Injae Shin*

Department of Chemistry, Yonsei University, Korea

Synthetic anion transporters have received attention as anticancer agents because of their potential to disrupt cellular ion homeostasis. However, a direct correlation between a change in cellular chloride anion concentrations and cytotoxicity has not been established for synthetic ion carriers. Here we show that calix[4]pyrrole based transporters induce coupled chloride anion and sodium cation transport in both liposomal models and cells, and promote cell death by increasing intracellular chloride and sodium ion concentrations. Removing either ion from the extracellular media or blocking natural sodium channels with amiloride prevents this effect. Cell experiments show that the ion transporters induce the sodium chloride influx, which leads to release of cytochrome c from the mitochondria and apoptosis via caspase activation. However, they do not activate the caspase-independent apoptotic pathway associated with the apoptosis-inducing factor. Ion transporters, therefore, represent an attractive approach for regulating cellular processes that are normally controlled tightly by homeostasis.

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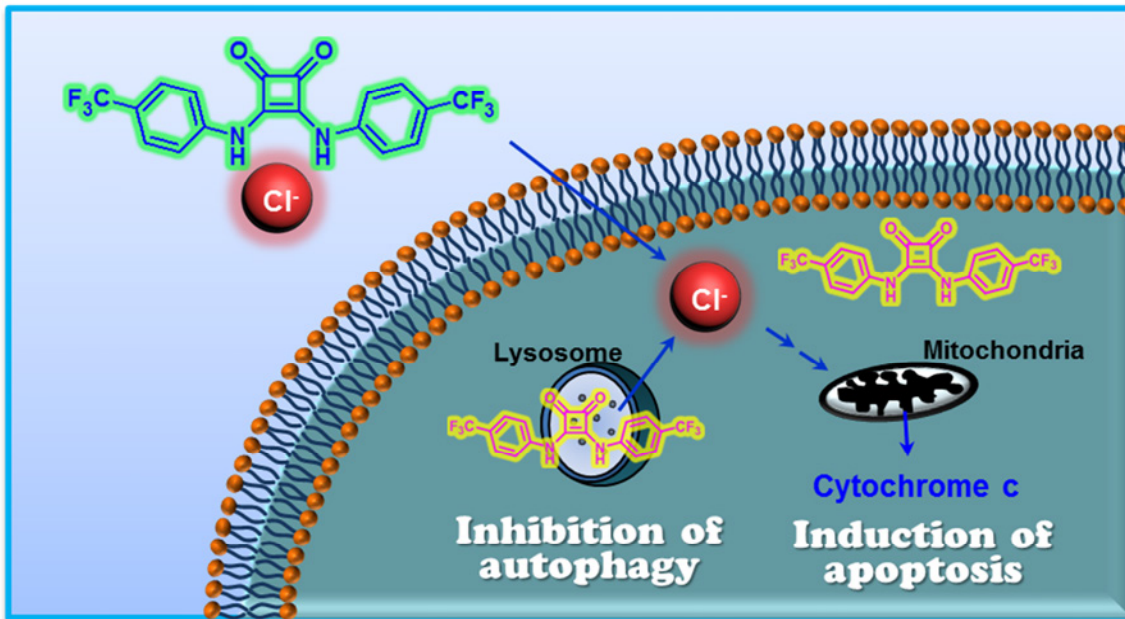
Type: Poster Presentation, Time: THU 11:00~12:30

A squaramide-based anion transporter disrupts autophagy and induces apoptosis by perturbing cellular ion homeostasis

Seong-Hyun Park, Injae Shin^{*}

Department of Chemistry, Yonsei University, Korea

Perturbations in cellular chloride concentrations can affect cellular pH and autophagy and lead to the onset of apoptosis. With this in mind, synthetic ion transporters have been used to disturb cellular ion homeostasis and thereby induce cell death; however, it is not clear whether synthetic ion transporters can also be used to disrupt autophagy. Here, we show that squaramide-based ion transporters enhance the transport of chloride anions in liposomal models and promote sodium chloride influx into the cytosol. Liposomal and cellular transport activity of the squaramides is shown to correlate with cell death activity, which is attributed to caspase-dependent apoptosis. One ion transporter was also shown to cause additional changes in lysosomal pH, which leads to impairment of lysosomal enzyme activity and disruption of autophagic processes. This study provides the first experimental evidence that synthetic ion transporters can disrupt both autophagy and induce apoptosis



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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design and Synthesis of Novel DYRK1B Inhibitors

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

Dual-specificity tyrosine-phosphorylation-regulated kinase (DYRK1B) has been known to play a key role for maintaining cells in quiescence, and its Amplification in various tumor types has been observed such as ovarian cancer, colon cancer, pancreatic cancer, and lung cancer, when compared to normal tissue [1]. Hence, many studies and development of DYRK1B inhibitors are actively in progress. We designed and synthesized novel DYRK1B inhibitors having potent enzymatic activities. Our data suggest therapeutic potential of DYRK1B inhibitors for the treatment of cancers.[1] *Bioorganic & Medicinal chemistry* 2015, 23, 4434-4441 *J. Med. Chem.* 2015, 58, 2834-2844

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Area: Medicinal Chemistry

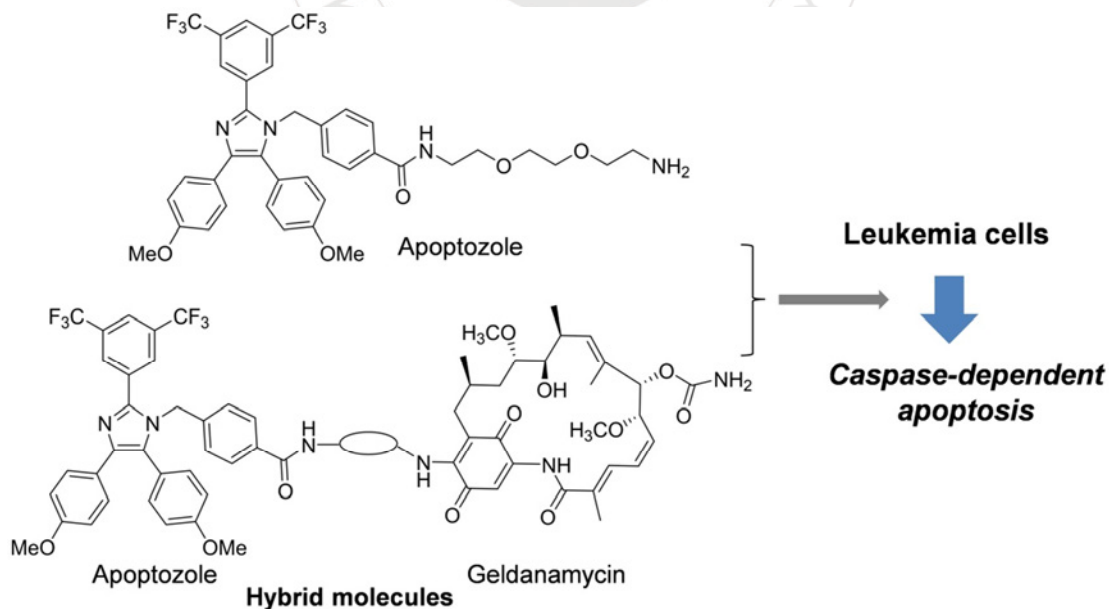
Type: Poster Presentation, Time: THU 11:00~12:30

Anti-leukemia activity of hybrid molecules of Hsp70 and Hsp90 inhibitors

Sang-Hyun PARK, Injae Shin*

Department of Chemistry, Yonsei University, Korea

To improve anti-leukemia efficacy of a small molecule inhibitor (apoptozole, Az) of Hsp70 proteins, Az was linked to Hsp90 (geldanamycin) or Abl kinase (imatinib) inhibitors. Hybrid of Az with geldanamycin significantly enhanced the anti-leukemia activity compared to individual inhibitors. However, hybrid of Az with imatinib showed lower cytotoxicity on leukemia cells compared to individual treatment. These findings suggest that hybrid of Az with geldanamycin could be utilized as potential anti-leukemia agents.



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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Validation of Carbonic Anhydrase-IX as a Target of Anticancer Using PET Imaging of [18F]-Acetazolamide

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¹*Korea Atomic Energy Research Institute, Korea*

Hypoxia is salient feature of broad numbers of solid tumors with more aggressive behavior leading poor prognosis, resistance to cancer treatments, increased metastasis and altered metabolism. Carbonic anhydrases (CA) are key enzymes involved in hypoxia induced stress, and regulated by transcriptional factor HIF 1/2 (hypoxia-inducible factor). Among 15 isozymes of CA, Carbonic anhydrase-IX (CAIX) a cell surface anchored enzyme is most prominently overexpressed in hypoxic condition. Overexpressed CAIX involved in several cancers as breast, lung, kidney, ovarian, brain, colon, head and neck cancers. Small molecules with sulfonamide pharmacophore are well known as CAIX inhibitor to achieve reduction of primary growth of cancers and distant metastasis. The clinically approved acetazolamide CAIX inhibitor is also emerged as promising biomarker for clinical imaging of CAIX expressing hypoxic tumors. The known acetazolamide biomarkers used for CAIX imaging are performed well predominantly for renal cancer cell line SKRC-52. Thus, further target validation of CAIX for development of clinically used biomarker is required to be performed. In this study, [18F] radioisotope was introduced to acetazolamide by CuAAC click to synthesize [18F]-Acetazolamide and imaging study was performed by PET in xenograft mouse model bearing 4T1 and HT-29 cell lines as well as metastatic tumor models.

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Anti-oxidative and anti-cholinesterase compounds from *Eisenia arborea*

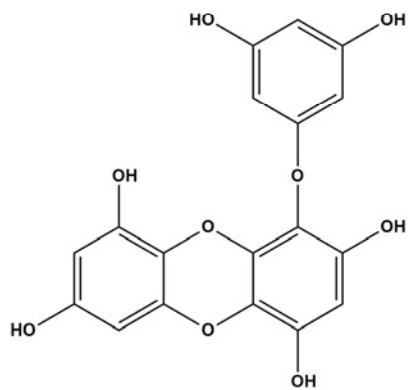
DaeYeoB Cho^{*}, Bong Ho Lee^{1,*}, Byong Wook Choi^{2,*}

Department of Chemical and Biological Engineering, Hanbat National University, Korea

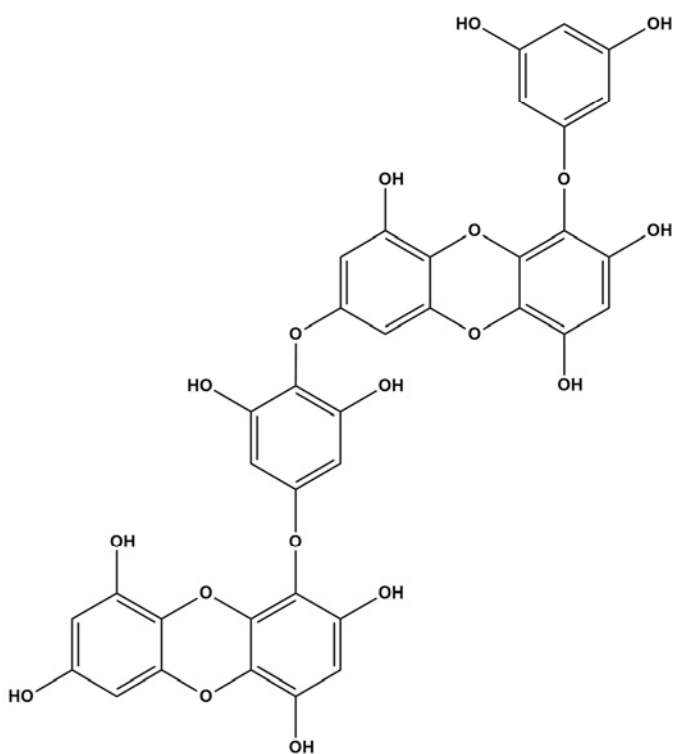
¹*Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea*

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In our continuing search for biologically active compounds from edible brown alga, *Eisenia arborea* was examined. Here we report the progress on the purification, biological activities and structural determination of the purified compounds. From the 100% methanol extract of *Eisenia arborea*, solvent partition fractions were prepared by using *n*-hexane(EAH), chloroform(EAC), butanol(EAB) and water(EAW). Among them EAB showed strong anti-oxidative, AChE* and BuChE** inhibitory and anti-tyrosinase activities. The EAB of *Eisenia arborea* showed 81.3% DPPH radical scavenging activity, 83.1% AChE inhibitory activity, 99.5% BuChE inhibitory activity and 75.3% tyrosinase inhibitory activity at 100 ppm. Using a series of ODS open column chromatography, four purified fractions, EAB-5, EAB-6 and EAB-8, EAB-9, could be obtained. At 100 ppm, they showed anti-oxidative activity as 72.1, 76.8, 67.5, 74.0%, anti-tyrosinase inhibitory activity as 66.3, 67.85, 91.3, 87.3% , and AChE inhibitory activity as 96.23, 98.99, 97.20, 96.07%, and BuChE inhibitory activity as 95.5, 97.9, 97.6, 98.0%, respectively. The major compounds of the purified fractions of EAB-5, EAB-6 and EAB-8, EAB-9 were determined by ¹H and ¹³C NMR and MS analysis. The compound EAB-5 and EAB-6 was turned out to be eckol whereas the compound from EAB-8 was turned out to be dieckol, respectively. The major compounds from EAB-9 are also to be discussed.*AChE : Acetylcholinesterase **BuChE : Butyrylcholinesterase



Eckol



Dieckol



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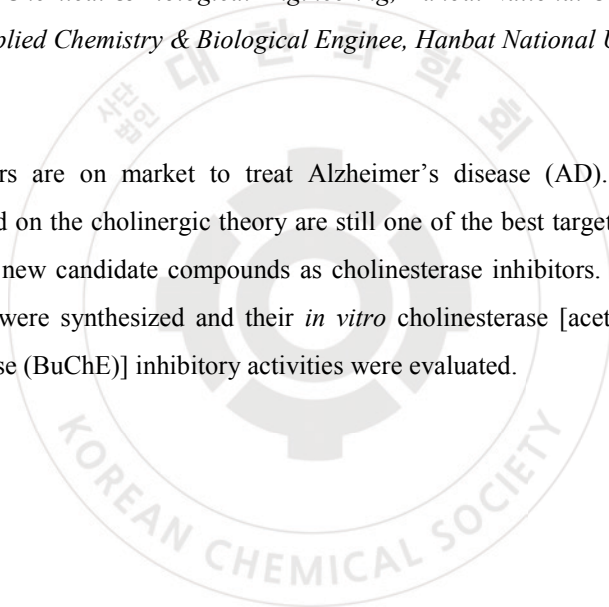
Tryptamine Derivatives for Novel Cholinesterase Inhibitors

Cheolmin Jeon^{*}, Jeong Ho Park^{1,*}, haneul lee, Yujung Kang

Department of Chemical & Biological Engineering, Hanbat National University, Korea

¹*Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea*

Cholinesterase inhibitors are on market to treat Alzheimer's disease (AD). Development of novel Alzheimer's drugs based on the cholinergic theory are still one of the best targets for AD. We have been researching to find out new candidate compounds as cholinesterase inhibitors. In this study, a series of tryptamine derivatives were synthesized and their *in vitro* cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated.



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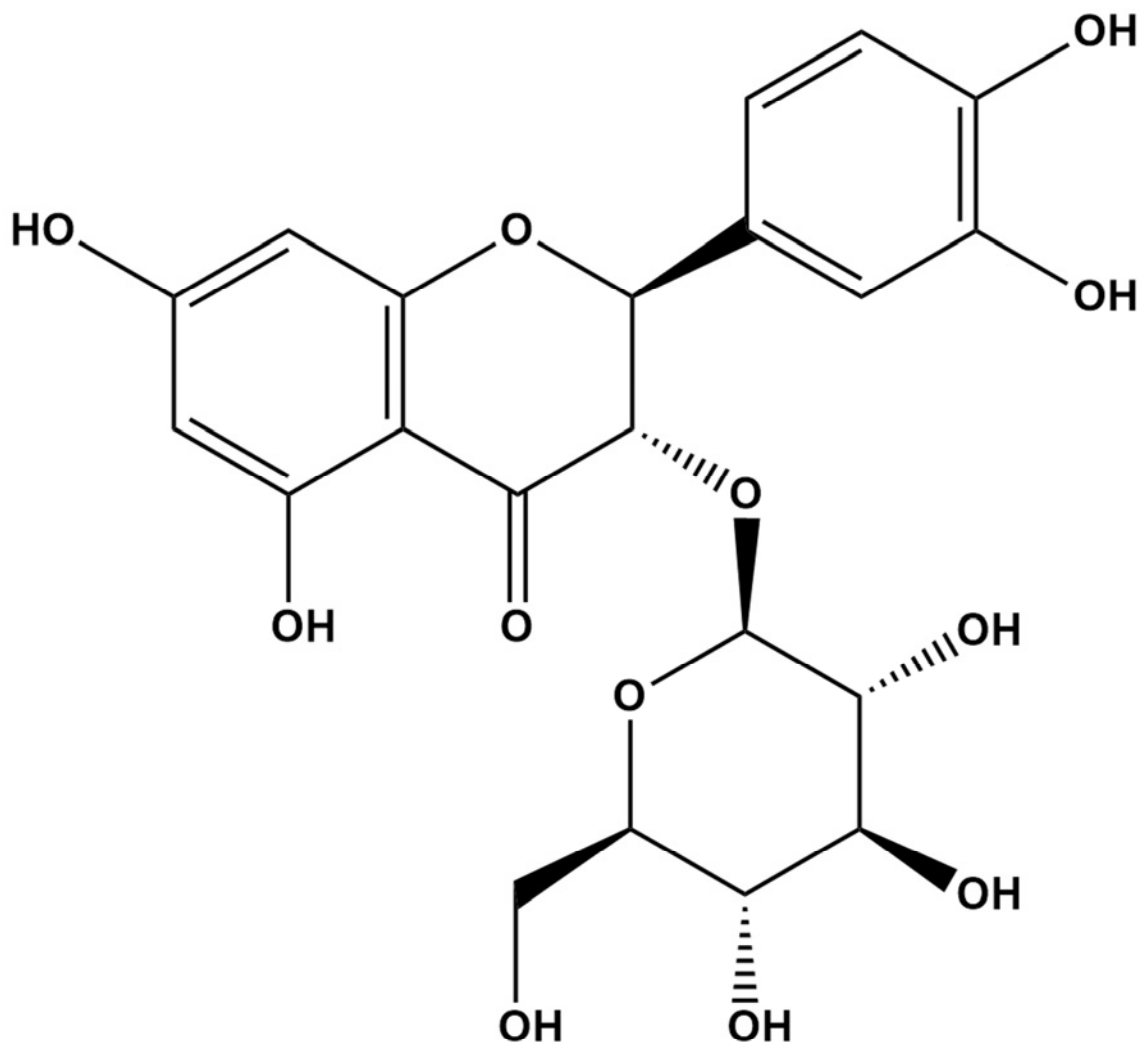
An anti-oxidative floavonol glucoside from *Agrimonia pilosa*

gyusun jeong^{*}, Heesu Kwon, Byong Wook Choi^{*}, Bong Ho Lee^{1,*}

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In our continuing search for anti-oxidative compounds from oriental medicinal plants, *Agrimonia pilosa* was examined. Here we report the progress on the purification, biological activities and structural determination of a compound from *Agrimonia pilosa*. From the 100% methanol extract of *Agrimonia pilosa*, solvent partition fractions were prepared by using *n*-hexane(15-APH), chloroform(15-APC), butanol(15-APB) and water(15-APW). Among them 15-APB showed anti-oxidative activity. The 15-APB of *Agrimonia pilosa* showed 53% DPPH radical scavenging activity at 100 ppm. Using a series of ODS open column chromatographic purification steps, one compound, 15-APB-175 was purified. At 100 ppm, it showed anti-oxidative activity of 92.3%. The structure of 15-APB-175 was determined using ¹H and ¹³C NMR and MS spectroscopic methods and its structure was turned out to be a floavonol glucoside named (2*S*, 3*S*)-glucodistylin.



(2S,3S)-Glucodistylin

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-343**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

New Reduced Asymmetric Xanthene Fluorescent Probes with Improved Chemical Stability and Reactivity: Application to Detection of Nitroreductase

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Department of Pharmacy, Suncheon National University, Korea

Xanthene fluorophores including fluorescein, rhodamine and their hybrid structure, rhodol, are among the most commonly used fluorescent probes, and many activity-based fluorescent probes have been discovered with their asymmetric derivatives in many areas including biology and medicines. Rhodol and rhodamine derivatives have been of great interest as activity-based fluorescent probes that can detect various phenomena in live cells because they are fluorescent with a high quantum yield within broad ranges of pH and are also known to be photo-stable as compared to other fluorescent probes such as fluorescein. However, as with other xanthene fluorophores, rhodol and rhodamine probes also have a synthetic disadvantage that it's difficult to modify and introduce various substituents at the terminal of xanthene ring due to low chemical stability to acids and bases. A few reduced xanthene fluorophores including fluorescein and rhodol have been developed, but the reduced asymmetric rhodamine fluorescent probe has not been discovered. Herein, we designed, synthesized and evaluated the reduced asymmetric xanthene fluorophores including fluorescein, rhodol and rhodamine moieties. In order to confirm synthetic advantage of reduced xanthene fluorophores, we evaluated chemical stability of reduced symmetric and asymmetric fluorophores by reacting them under alkylation and amide coupling reaction conditions. Additionally, we performed the study for evaluation of fluorogenic nature of reduced fluorophores. Nitroreductase (NTR)-, which is a representative biomarker of hypoxia, response fluorescent probes were synthesized with these reduced fluorophores, and their fluorescent activities were evaluated in presence of NTR.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-344**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Identification of Novel 2,4-diaminopyrimidines bearing fused tricyclic ring moiety as potent anaplastic lymphoma kinase (ALK) inhibitor with in vitro, in vivo Antitumor activity

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In this study, a series of novel 2,4-diaminopyrimidines bearing fused tricyclic ring moiety was described for ALK inhibitor. The pyrazole, imidazole, 1,2,4-triazole, piperazine and phenanthridine moieties were employed at the 2-position of pyrimidine. Among the compounds synthesized, 28, 29, 36, and 42 showed promising anti-ALK activities in enzymatic- and cell-based assays. In vivo H3122 xenograft model study showed that compound 29 effectively suppressed ALK-driven tumor growth, similar to the extent of ceritinib, suggesting that it could be used for a novel ALK inhibitor development.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-345**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of biomarkers that fluoresce by binding with TTR

SeokBeom Lee, yerim jung, AhReum Han, Sungwook Choi*

Development of Drug Development and Discovery, Chungnam National University, Korea

Transthyretin (TTR) is a transport protein in the serum and cerebrospinal fluid (CSF) that carries the thyroid hormone thyroxine (T4) and retinol-binding protein bound to retinol. Each monomer is a 127-residue polypeptide rich in β -sheet structure. TTR is one of the Amyloid- β ($A\beta$) binding proteins and prevents its aggregation and fibrillation. $A\beta$ aggregation is known to cause Alzheimer's disease (AD). AD has no mechanism and treatment yet and should manage through early diagnosis. According to the reported paper, cerebrospinal fluid (CSF) and plasma TTR levels were significantly lower in Alzheimer's patient. Therefore serum TTR level has tremendous potential as one of the noninvasive diagnostic and prognostic biomarkers. Thus, we synthesize a low-molecular compound that selectively reacts with Lysine-15 in a thyroxine binding pocket of TTR to design a biomarker for early diagnosis of AD.

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Code: **MEDI.P-346**

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Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-347**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Inhibitors of TTR amyloidogenesis and fluorescent probes based on 3H-Indole platform

Hye Rim Lim, Seo Yun Kim, Sungwook Choi*

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Transthyretin(TTR) is a homotetrameric protein composed of 127-amino-acid, β -sheet-rich subunits. The established physiological functions of TTR are to bind to and transport the thyroid hormone thyroxine (T4) and holo-retinol binding protein in the blood and cerebrospinal fluid (CSF). TTR is one of the A β -binding proteins and generating amyloid fibrils. This protein binds to A β and prevents A β aggregation and fibrillation. Consequently, TTR inhibits A β -induced cellular toxicity that associated with Alzheimer's disease(AD). AD is chronic neurodegenerative disease, and is the cause of 60% to 70% of cases of dementia. According to the reported paper, CSF and plasma TTR levels were significantly lower in alzheimer's patient. Therefore serum TTR has tremendous potential as one of the noninvasive diagnostic and prognostic biomarkers. So herein , We synthesized compounds and evaluated their ability as a TTR fluorescent sensors and sufficient inhibitors of TTR amyloidogenesis.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-348**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Studies for relationship between proteins and topological water network using MD simulation of natural amino acids and crystal water analysis for all PDBs

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Water plays an important role in protein stability, folding, function, and ligand binding. Protein hydration has been studied using free energy perturbation algorithms such as WaterMap, SZMAP, and GIST. However, free energy calculations are difficult to carry out as well as time consuming. In this work, topological water network (TWN) analysis was used instead of free energy calculation. TWN is defined by various hydrogen bond geometry formations such as 3-, 4-, 5-, and 6- water rings. Twenty natural amino acids were capped with N-methylamide (NME) and acetyl (ACE) groups on C- and N-terminals, respectively to avoid charge effects. TWN of each amino acid was analyzed by molecular dynamics (MD) simulation using GROMACS software. Conformers of the capped amino acids obtained from MD simulations were analyzed through Ramachandran plots. MD simulation results showed that non-polar atom (C) of hydrophobic amino acids like ALA and ILE was located at the minimal distance from the water ring. However, polar atoms (O and N) were found to be closest to the water ring in case of hydrophilic amino acids like SER, GLU, and ARG. In addition to MD simulation of each amino acid, water molecules from all PDBs were extracted by an in-house program and TWN was analyzed. Similar to MD simulation results, TWN was located around polar atoms (O and N) in hydrophilic residues while in case of hydrophobic residues it was found around non-polar atom (C). Findings of this study could be exploited for TWN-based drug discovery and development.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-349**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and biological evaluation of niclosamide derivatives as Wnt/ β -catenin inhibitor

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The Wnt signaling pathway has a critical role in regulation of tissue homeostasis and organ development. Dysregulated Wnt activity is one of the major underlying mechanisms responsible for many diseases including cancer. Recently, few results published regarding the FDA-approved anthelmintic drug Niclosamide inhibits Wnt/ β -catenin signaling and suppresses colon cancer cell growth in vitro and in vivo. Niclosamide is a multi-functional drug that possesses important biological activity in addition to inhibition of Wnt/ β -catenin signaling. Here, we studied the SAR of Wnt signaling inhibition in the salicylamide region of Niclosamide. We found that the 5-chloro-2-methoxybenzenesulfonamide can be effectively inhibit tumor growth. With this result, we synthesized several derivatives as Wnt/ β -catenin inhibitor.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-350**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Enterovirus Inhibitory Activity of substituted Urea and Thiourea derivatives of p-Benzene sulfonamide

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

A series of substituted Urea, Thiourea and amide derivatives of p-Benzene sulfonamide were prepared with one or two methylene group/s as linker between them. These were tested for their inhibition property against HRV-A and HRV-B. Some of the compounds synthesized have sub-micro molar range of activity against HRV 21 and HRV 71 and moderate activity against HRV 14 with low cytotoxicity and high selectivity index values. Initial time of addition experiments shows that this might be a capsid binding inhibition.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-351**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Discovery of novel autotaxin inhibitors using molecular docking studies

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Autotaxin (ATX) has been associated with breast, thyroid, prostate, lung and ovary cancers. Besides, it is involved in chronic fibrotic diseases of lung, eye, kidney and liver. Accordingly, ATX is a promising target for the design and development of the novel anticancer and antifibrotic agents. In an effort to discover novel highly potent ATX inhibitors, we designed a series of ATX inhibitors using molecular docking studies. Additionally, docking studies inside the active site of ATX shed light on their binding mode and interactions. These compounds were further synthesized and evaluated for their inhibitory activities against ATX. Docking results also assisted in the examination of structure-activity relationship (SAR). 4-([4-(4-phosphonomethyl-phenyl)-thiazole-2-carbonyl]-amino)-piperidine-1-carboxylic acid 3,5-dichloro-benzyl ester was found to be the most potent compound of this series. It showed higher potency than already known ATX inhibitors. Overall, this work offers a promising ATX inhibitor for further evaluation and development.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-352**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

New Substituted Quinazolinedione Derivatives as Potential DDR1 Kinase Inhibitors

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²*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

The aims from this study are to design and synthesize new hit antiproliferative compounds with novel scaffolds able to inhibit the oncogenic DDR1 kinase. In this study, fifteen quinazolinedione scaffold-derived compounds were designed, synthesized and evaluated as potential DDR1 inhibitors. Eight compounds exhibited very weak inhibitory activity for DDR1 kinase namely 2.6a, 2.6d, 2.6e, 2.6f, 2.7c, 2.7d, 2.7g and 2.8a. Three compounds showed weak inhibitory activity namely 2.6b, 2.7e and 2.7f. Moderate activity has been exerted with compounds 2.6c, 2.7a and 2.7b with percent inhibition of 29.18%, 27.53% and 22.61%, respectively. Surprisingly, compound 2.6g showed the highest inhibitory activity over DDR1 kinase with %inhibition of 70.20%. Structure activity relationship (SAR) study has been carried out and suggested substituent position affects the inhibitory effect. In addition, kinase selectivity panel for the most active compound 2.6g has been performed. The result showed compound 2.6g selectively inhibits DDR1 kinase.

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Code: **MEDI.P-353**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of 4-alkyl-6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-e][1,2,4]triazolo[4,3-a]pyrimidin-5(4H)-ones as Non-capsid Enterovirus Inhibitors with Enhanced Pharmacokinetic (PK) Properties

Yashwardhan Malpani, Young-Sik Jung^{1,*}, SOO BONG HAN²

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In continuation of our ongoing research on 4-aryl-6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-e][1,2,4]triazolo[4,3-a]pyrimidin-5(4H)-one derivatives as anti-enteroviral compounds, we prepared 4-alkyl-6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-e][1,2,4]triazolo[4,3-a]pyrimidin-5(4H)-one analogs and tested them against representative enteroviruses including Human Coxsackievirus B1 (Cox B1), Human Coxsackievirus B3 (Cox B3), human Poliovirus 3 (PV3), human Rhinovirus 14 (HRV14), human Rhinovirus 21 (HRV 21) and human Rhinovirus 71 (HRV 71). Some of the N-4-alkyl derivatives showed remarkable improvement in the activity (selectivity indices) especially against rhinoviruses and poliovirus species. Among the prepared compounds, N-4-propyl derivative showed single digit micromolar activities (1.6-2.0 μM) against tested HRV's and PV3 with improved selectivity index (SI) values (16.1-59.9). The N-4-propyl derivative also showed improvement in other pharmacokinetic properties when compared with the best compound in earlier series (N-4-phenyl derivative) such as less cytotoxicity, high metabolic stability (human) and better logP/ClogP values. The N-4-propyl derivative also behaved better in CYP & in-vivo PK (Rat) assays and thus overall has more drug likedness character. Preliminary mode of action studies reveal that these compounds are not capsid inhibitors of enteroviruses but instead they acts in later stage/s of virus replication cycle.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-354**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The development of antiviral agent for Hepatitis B virus

kyuneun kim, SOO BONG HAN^{*}, Young-Sik Jung

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Hepatitis is a word derived from *hepar*, meaning 'liver' and *-itis*, meaning 'inflammation', which causes inflammation in the liver. The number of chronic infections is around 300 million people worldwide, and the number of deaths per year is 600,000. In order to cure HBV fundamentally, it is necessary to inhibit cccDNA formation. However, since there is no definite cccDNA inhibitor known, therapies that target other parts of HBV life cycle have been developed and used. Currently developed therapies have several disadvantages, therefore necessitating other alternatives. In this study, the aim is to develop capsid inhibitor, which impedes the capsid assembly during the lifetime of the HBV life cycle. Based on the structure of the existing capsid candidate, they designed, synthesized, and evaluated their pharmacological activity. As a result, candidate materials showing notable pharmacological activity were found.

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Code: **MEDI.P-355**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Histone Deacetylase 6 (HDAC6) inhibitors for anti-cancer drug and its implication for cancer therapy

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Histones are primary protein components of chromatin that compact the DNA. Acetylation of histones by HATs is related with genes transcription while Deacetylation of lysine residue of genes for compensation is related with gene silencing. HDACs are classified into class I, class II, class III and class IV groups based on their sequence homology. Classical HDACs are Zn²⁺-dependent enzymes are having a catalytic pocket with a Zn²⁺ ion at its base that can be inhibited by Zn²⁺ chelating compounds such as hydroxamic acids. Its function includes transcriptional regulation, cell cycle progression and developmental events. Anomalous histone deacetylase (HDAC) activity is common in acute myeloid leukemia. HDAC inhibitors draws more attention of inventors in recent years because of its promising anti-cancer activities. Until now, many HDAC inhibitors reached clinical trial, and some of them are approved for clinical uses such as Ac-lysine, SAHA, FK228, PXD101, LBH589, etc. Here we present the design, synthesis and biological activities of disubstituted phenyl N-hydroxy propanamide.

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Code: **MEDI.P-356**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Novel FMS inhibitors based on pyrimidine scaffold with improved selectivity and cellular activity

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FMS (Feline McDonough Sarcoma oncogene) is a type III receptor tyrosine kinase belonging to the PDGFR (Platelet-derived growth factor receptor) family. FMS is overexpressed in certain type of cancers including myeloblastic leukemia and bone carcinoma. Our team had developed compound 1 as a potent FMS inhibitor with excellent selectivity profile but lacking satisfactory cellular activity. The structure of compound 1 was modified using medicinal chemistry tools and a series of compounds was synthesized aiming at improving the cellular activity while keeping the potency and selectivity. The whole series was assayed over FMS kinase as well as a panel of 13 other kinases to assess the potency side to side with the selectivity. Compound 2 showed the highest potency over FMS kinase and excellent selectivity profile. Compounds 1 and 2 were assayed over M-NFS-60, U2OS cell lines and NCI-60 cell lines panel and compound 2 showed much better inhibitory profile than compound 1.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of Histone Deacetylase (HDAC) inhibitors

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Today, people suffer from many kinds of disease. From the World Health Organization (WHO) statistics in 2012, the top 10 killers, many of which are lifestyle-related, account for 51.4% of all deaths globally. Especially cancer was ranked the fifth place about death caused by an illness. For this, many cancer inhibitors have developed chemotherapy. The anti-cancer drugs have caused troubles from side effect, so institutions have been studying on targeted cancer drugs for intensive treatment such as HDAC inhibitors. Histone deacetylases (HDACs) are enzymes which determine gene expression. The acetylation of histones is balanced by histone acetyltransferases (HATs) and histone deacetylase (HDACs). HDACs remove the acetyl group of lysine residues in histone tails and associate with a more condensed chromatin state. It also suppresses gene expression with tumor genes. While HATs acetylate on lysine residues in histone tails and associate with a more relaxed chromatin state and gene-transcription activation. HDACs have become promising targets in recent years for cancer therapy, but there are still few inhibitors showing high target selectivity. Some of medicines for HDAC inhibitors, which are Vorinostat, Romidepsin, Belinostat and Panobinostat were approved by the U.S FDA. In this study, we designed and synthesized HDAC inhibitors. These compounds were investigated for their HDAC inhibitory actions and in vitro anti-tumor activities against cancer cell.

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Code: **MEDI.P-358**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design and Synthesis of Novel Checkpoint inhibitors of PD-1/PD-L1 Pathway

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The protein PD-1 (Programmed Death-1) belongs to the CD28 family and is an inhibitory receptor. It is expressed at the surfaces of various immune cells including activated T-cells, B lymphocytes, dendritic cells, monocytes, and macrophages. PD-L1 expression in various tumors is driven by oncogenic signaling pathways (e.g., PI3K/AKT, ALK, and STAT-3 pathways). When PD-L1 binds to PD-1, an inhibitory signal is transmitted into the T cell, which reduces cytokine production and suppresses T-cell proliferation. Tumor cells exploit this immune-checkpoint pathway as a mechanism to evade detection and inhibit the immune response. In immuno-oncology, small-molecule drug discovery targeting PD-1/PD-L1 and IDO1 has rapidly evolved into an important research area. As small molecule drugs have several advantages over monoclonal antibodies, such as high feasibility, oral bioavailability, and access to intracellular disease targets, pharmaceutical industries are working on small molecule drugs for PD-1/PD-L1. BMS-202, developed by Bristol-Myer-Squibb, is a novel inhibitor of PD-1/PD-L1 complex formation, which is currently undergoing clinical phase I trial for the treatment of lung, renal cell carcinoma, Hodgkin lymphoma cancers. Herein, we present the design and synthesis of novel small molecules as PD-1/PD-L1 inhibitors.

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Area: Medicinal Chemistry

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Synthesis and biological evaluation of N9-cis-cyclobutylpurine derivatives for use as cyclin-dependent kinase (CDK) inhibitors

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A novel 6-aminopurine scaffold bearing an N9-cis-cyclobutyl moiety was designed using structure-based molecular design based on two known CDK inhibitors, dinaciclib and Cmpd-27. A series of novel 6-aminopurine compounds was prepared for structure-activity relationship (SAR) studies of CDK2 and CDK5 inhibitors. Among the compounds synthesized, compound 81 displayed potent CDK2 and CDK5 inhibitory activities with low nanomolar ranges ($IC_{50} = 2.1$ and 4.8 nM, respectively) and showed moderate cytotoxicity in HCT116 colon cancer and MCF7 breast cancer cell lines. Here, we report the synthesis and evaluation of novel 6-aminopurine derivatives and present molecular docking models of compound 81 with CDK2 and CDK5.

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Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Construction of Diazepine Derivatives using Solid-phase Synthesis

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Solid-phase organic synthesis has become an important technology for the construction of chemical libraries for several years. The construction of chemical library is necessary to search of drug-like compound and solid-phase synthesis can be used usefully. Diazepine moiety has been widely used in pharmaceutical industry. Among of diazepine derivatives, 1,4-diazepine-2,5-diones, which are privileged scaffolds, and its fused-heterocycles play an important role in the area of drug discovery and medicinal chemistry. For examples, 3,4-dihydro-1H-benzo[e][1,4]diazepine-2,5-dione have been developed histone deacetylases inhibitors (HDAC), antileishmanial agent, angiotensin converting enzyme (ACE) inhibitors, acyl CoA : monoacylglycerol acyltransferase2(MGAT2) inhibitor, melanocortin receptor agonists, cholinesterase inhibitors. Owing to these properties, many synthetic methods for 3,4-dihydro-1H-1,4-diazepine-2,5-diones fused heterocycle such as pyridine, pyrrole, imidazole, pyrazole, thiophene, isothiazole, furan, and thiadiazole have been well reported. Previously, we reported thiazoles and their fused-heterocycle libraries using traceless solid-phase synthesis. Our current interest in small-molecule library based on fused-thiazole scaffolds prompted us to the synthesis of 4H-thiazolo[4,5-e][1,4]diazepine-5,8-dione derivatives.

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Code: **MEDI.P-361**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

1,2,3-Triazoloamide Derivatives Using Solid- and Solution-Phase Synthetic Approaches

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A secondary 1,2,3-triazoloamide library was constructed and expanded by a previously developed solid-phase synthetic route and a tertiary 1,2,3-triazoloamide library was constructed by a parallel solution-phase synthetic route. The target secondary and tertiary 1,2,3-triazoloamide derivatives were obtained with three-diversity points in excellent overall yields and purities using the reported solid and solution-phase synthetic routes, respectively. This investigation, has led to the development of the solid- and solution-phase route for the synthesis of various 1,2,3-triazoloamides that contain three diversity sites that were introduced in reactions involving amines (R1 and R2), chloro-acid chlorides (A), and terminal acetylenes (R3). The strategy allows for a ready access to a large library and is potentially applicable to the preparation of other 1,2,3-triazole derivatives.

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Code: **MEDI.P-362**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Novel Functionalized Amino Acid Derivatives as MAO-B Inhibitors for Alzheimer's Disease Therapy

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Alzheimer's disease is a progressive and neurodegenerative disorder which involves multiple molecular mechanisms. In AD, reactive astrocytes aberrantly and abundantly produce the inhibitory transmitter GABA by over-expressed monoamine oxidase-B(MAO-B). GABA is the major inhibitory transmitter in the brain and is released not only from a subset of neurons but also from glia. Based on this novel target, we developed a lead compound, KDS2010, which showed potent and selective inhibitor of aberrant GABA synthesis and excellent drug-like properties in ADME/Tox. Thus we plan to evaluate KDS2010 for a pre-clinical candidate, which will serve as an effective treatment for memory impairment in Alzheimer's disease by targeting aberrant GABA synthesis in reactive astrocytes. In this study, we synthesized a modified series of functionalized amino acids (FAAs) for backup compounds of KDS2010. KDS5001 showed potent and selective MAO-B inhibitory activity (IC₅₀ of human MAO-B = 4 nM, selectivity against MAO-A: > 10,000) and good reversibility compared with selegiline, well-known irreversible MAO-B inhibitor. In addition, it exhibited favorable in vitro ADME/tox profile.

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Code: **MEDI.P-363**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Evaluation of Mn-EDTA-EOB Conjugate as a new Hepatobiliary MRI Contrast Agent

**KAMRUL ISLAM, Hee Kyung Kim¹, Soyeon Kim, Choi Garam, Ah Ruem Baek,
BoKyung Sung, Byeong Woo Yang, Seong hwan Hwang², Yongmin Chang^{3,*}**

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Magnetic resonance imaging (MRI) is one of the best noninvasive diagnostic modality in medical imaging. Gadolinium (Gd) complexes are widely used as longitudinal (T_1) contrast agents (CAs). However, administration of Gd-based MRI CAs can generate serious side effects such as nephrogenic systemic fibrosis (NSF) in some patients. Mn(II) has five unpaired electrons, slow electron relaxation, fast water exchange kinetics and lower intrinsic toxicity than Gd^{3+} , which makes it an attractive alternative of gadolinium(III) for enhanced MRI applications. we design and synthesis a novel Mn^{2+} complex based on an ethylenediaminetetraacetic acid (EDTA) coordination cage bearing an ethoxybenzyl (EOB) moiety with high chelation stability for use as a hepatobiliary agent. Also, we measured the magnetic and kinetic properties of Mn-EDTA-EOB complex in comparison, and liver and bile excretion pattern was confirmed through *in vivo* MR images, along with biodistribution of Mn-EDTA-EOB.

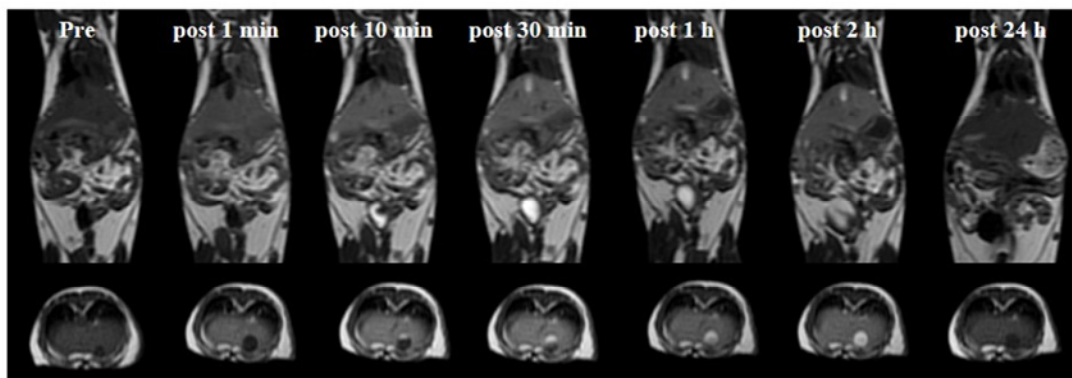
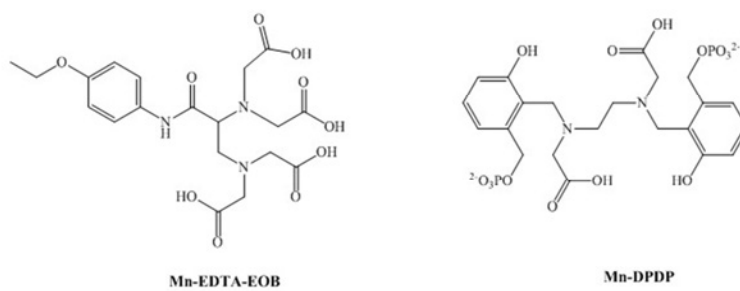


Figure 1. Structures of Mn-EDTA-EOB and Mn-DPDP and *In vivo* images of Mn-EDTA-EOB.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-364**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

SYNTHESIS AND BIOLOGICAL EVALUATION OF CHALCONE DERIVATIVES AS NEUROPROTECTIVE AGENTS FOR NEUROLOGICAL DISORDERS

Hyeon Ji Kim, Ki Duk Park*

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Although the etiology of Parkinson's disease (PD) is unclear, recent reported studies suggest that oxidative stress contributes to the cascade leading to dopaminergic (DAergic) neurodegeneration. 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 antioxidant enzyme genes. We have synthesized novel chalcone derivatives to improve their Nrf2 activity and ADME/Tox profiles. Among the derivatives, compound 12d showed significant efficacy for activating Nrf2 and excellent profiles in ADME/Tox tests. In addition, compound 12d effectively protected DAergic neurons and attenuated PD-associated behavioral deficits in the MPTP-induced mouse model.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-365**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Biological evaluation of Benzothiazole aniline (BTA) Derivatives and their Platinum Complexes as antitumor agents

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Success of the cisplatin paved the way for second and third generation platinum drugs such as carboplatin, oxaliplatin. However, novel platinum agents still appeal much attention for the reason that drug resistance and several disadvantages, particularly related to general toxicity which lead to undesirable side effects are often detected with the current Pt based drugs. Benzothiazole aniline (BTA) is a potent and selective antitumor agent, displayed characteristic profile of cytotoxic response towards various tumor cell lines, whereas no hormonal dependency was identified. Since 1996 a series of benzothiazole derivatives based on the core compound benzothiazole aniline (BTA) have been established as anticancer agents. Also, ring-substituted derivatives of benzothiazole aniline was developed as antitumor agent and one derivative phortress (NSC 710305) was approved for phase 1 clinical trials as the prodrug. One approach to design novel Pt complexes to attach the platinum coordination moiety with an appropriate carrier ligand which selectively target the cancer cells. Based on the above approach, we design novel ligands L1, L2, L3 and their platinum complexes PtL1, PtL2, PtL3 by conjugate BTA moiety with three different type of Pt (II) coordination cage via amide bond to generate complexes with two active sites on the metal core. (Figure 1) Here in we report, the synthesis, structural characterization and in vitro cytotoxicity of this novel BTA derivatives and their platinum complexes to use as selective anticancer agents. We hypothesize that, tumor selectivity of this novel compounds were mainly driven by the lipophilic nature of BTA. Except PtL3 all other compounds show higher cytotoxicity than commercially available platinum drug cisplatin.

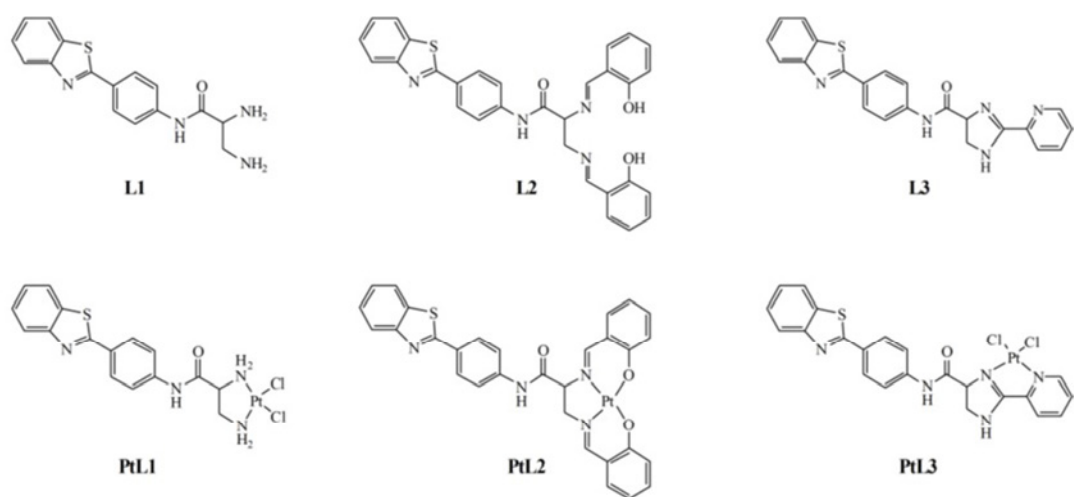


Figure 1. Structures of BTA derivatives **L1**, **L2**, **L3** and platinum complexes **PtL1**, **PtL2**, **PtL3**.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-366**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

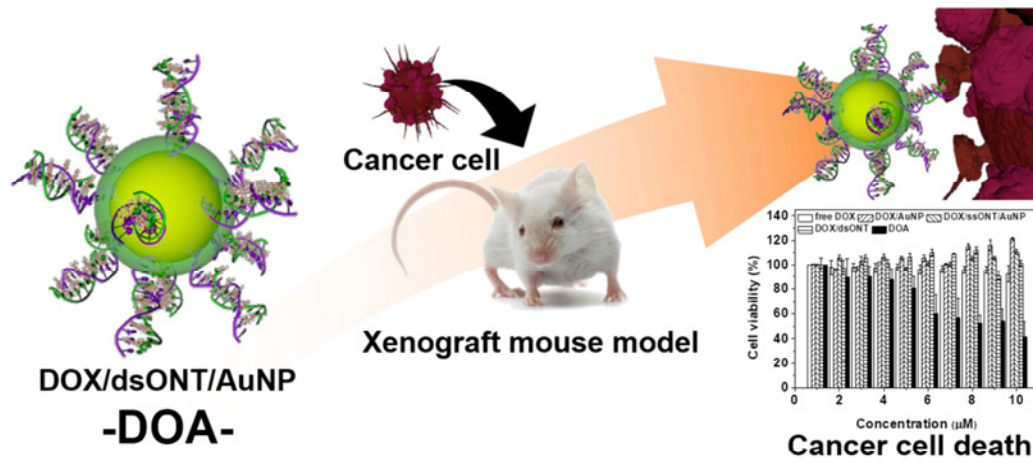
Drug delivery with doxorubicin loaded oligonucleotide modified gold nanoparticles for colorectal cancer treatment

Chang-Seuk Lee, SuHwan Yu¹, Tae Hyun Kim^{*}

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¹*Chemistry, Soonchunhyang University, Korea*

In this study, we propose doxorubicin (DOX) loaded oligonucleotides (ONTs) modified gold nanoparticles (AuNP) as a drug delivery system (DDS) for colorectal cancer therapy. DOX is one of representative anti-cancer drug and widely used by many research groups as a chemotherapy agent in the DDS. We utilized AuNPs as drug delivery vehicle, because of the advantages of AuNPs such as simple steps in synthesis, high surface-area-to-volume ratio, and biocompatibility. AuNPs were synthesized to be 13 nm diameter by conventional chemical reduction with citrate stabilizer. The G-C rich ONTs were used both for drug loading sites and AuNPs capping materials. The drug loading capacity of DOX loaded ONTs modified AuNPs (DOA) was represented by drug loading content (LC, w/w%), and drug entrapment efficiency (EE, %). The LC and EE of DOA was calculated as 3.02 and 81, respectively. The SW480 cell line was obtained as targeting system of colorectal cancer therapy. The cytotoxicity effect on SW480 cells treated with DOA was performed at in vitro (MTT assay) and in vivo (tumor-bearing mouse). The cell viability of SW480 that treated with DOA for 24 hours, was 41.77 %. The tumor growth inhibition ratio was represented by treatment-control (T/C) ratio; the T/C ratio was found to be 0.69. Thus, our results suggest the use of DOAs as promising drug delivery systems for colorectal cancer therapy.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MEDI.P-367**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and biological evaluation of guggulsterone derivatives as kidney cell protective agents

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We synthesized guggulsterone derivatives using [3+2] click reaction with aryl and alkyl acetylene with relatively high yields. These synthesized derivatives were evaluated for kidney cell protection effects against cisplatin toxicity. cisplatin is known as anticancer agent. However, cisplatin induced severe side effects to kidney cells by increasing oxidative stress. Therefore, cisplatin treatment is generally used for chronic kidney disease model. In this research, we evaluated kidney cell protective effects of guggulsterone derivatives. Among these guggulsterone derivatives, 6g which has hydroxyl group show protection effects. It is known that cellular oxidative stress induces MAPK kinase signal pathway and caspase activation. We therefore investigated if 6g reduces these signal cascades. We further investigate population of live of dead cells after treatment of 6g. These data indicated that inhibition of the mitogen-activated protein kinase/caspase-3 signaling cascade by 6g mediates its protective effects against cytotoxicity in cultured LLC-PK1 kidney cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-368**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Insights of a Lead Optimization Study and Biological Evaluation of Novel 4-Hydroxytamoxifen Analogs as Estrogen-Related Receptor γ (ERR γ) Inverse Agonists

Jina Kim, Sung Jin Cho*

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

Estrogen-related receptor γ (ERR γ) has recently been recognized as an attractive target for treating inflammation, cancer, and metabolic disorders. We 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 agonists for ERR γ but also exhibited enhanced pharmacokinetic profile compared with GSK5182. The newly synthesized GSK5182 analogs had comparable potency to GSK5182 and were far more selective for ERR γ over the ERR α , - β , and ER α . The in vivo pharmacokinetic profiles were further evaluated, as they possessed superior in vitro ADMET profiles compared to the other compounds. Additionally, it was reported that GSK5182 facilitates the responsiveness to radioiodine therapy by modulating sodium iodide symporter (NIS) function in anaplastic thyroid cancer (ATC) cells through the ERR γ and MAP kinase signaling pathway. Thus, GSK5182 derivatives possess advantageous druglike properties and can be used to potentially treat various ERR γ -related disorders.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-369**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of novel multi-chelator tether for mAb radiolabeling

Hyeonsu Na, Heejung Kim¹, ILJUNG LEE^{1,*}, Eunbi Shin¹, Dong Wook Kim^{*}, Jai Woong Seo²

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¹*Korea Institute of Radiological & Medical Science, Korea*

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Bioorthogonal chemistry has been exploited in tagging diverse biomolecules such as intra/intercellular or membrane proteins. Non-invasive in vivo immune-PET (Positron Emission Tomography) has also been benefited by advanced labeling methods derived from bioorthogonal chemistry. The specific activity of monoclonal antibody (mAb) relies on the number of radiometal chelator conjugated on mAb. Although several number of amine or cysteine on mAb can be functionalized with NHS- or maleimide-chelator, there are limited number of available amines for radiolabeling. High chelator/mAb ratio often impedes an intact binding avidity by blocking the functional amine on mAb. Here we designed and synthesized mAb conjugated with multiple chelators, called multi-chelator tether, via inverse electron demand Diels-Alder(IEDDA) reaction. Multi-chelator tether may increase the specific activity of radiolabeled mAb without depleting available amines on the mAb and provide a high target signal to background ratio in tumor mouse model.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-370**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A new method for conjugation of a photosensitizer to a natural plant phenolic food additive

HWAN SUK LEE, Yong-Wan Kim^{1,*}

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¹*Dongsung BioPharm, Korea*

Photodynamic therapy (PDT) involves the combination of non-toxic dyes known as photosensitizers (PSs) and visible light of the correct wavelength to be absorbed by the PSs. To improve the efficiency of intracellular delivery of photosensitizers and the efficacy of antitumor effect of photodynamic therapy, chlorin e6 and curcumin were conjugated with hydrophilic and hydrophobic linkers. Recognition and exploitation of the mechanistic aspects will be discussed in the presentation.[This study was supported by a grant of the Daegu-Gyeongbuk Medical Innovation Foundation Medical Device Development Center R&D Project(DG15D001)]

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MEDI.P-371**

Area: Medicinal Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Novel photosensitizers for photodynamic therapy(PDT) based on aggregation induced emission enhancement(AIEE) and thermally activated delayed fluorescence(TADF)

jaemoon lee, Jae Pil Kim^{1,*}

Department of Material Engineering, Seoul National University, Korea

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

The hydrophobic nature of conventional photosensitizers makes it difficult for PSs to disperse and even causes PSs to aggregate in aqueous physiological environment. In aggregates, the planar structure of PSs maximizes the π - π intermolecular interactions and thus greatly contributes H-aggregation which reduces efficiencies of fluorescence and singlet oxygen generation, namely aggregation caused quenching(ACQ). To address this problem, considerable attention has been focused on aggregation induced emission enhancement(AIEE) in photoluminescence research area. Unlike aggregation caused quenching, by their unique rotating geometry, AIE(E) aggregates exhibit high fluorescence with increasing concentration, even in aqueous physiological environment. Aggregation induced photodynamic therapy enhancement(AIPE) inspired by AIE(E) has been studied last two years and several groups showed AIPE photosensitizers could be a promising therapeutic strategy for photodynamic therapy. Our group synthesized novel photosensitizers based on boron dipyrromethane(BODIPY) derivatives and confirmed aggregation induced photodynamic therapy enhancement(AIPE) and emission enhancement(AIEE) of these photosensitizers. Triphenylamine(TPA) moieties were introduced on a BODIPY core for an AIPE and thermally activated delayed fluorescence(TADF) phenomena. The high-angle between donor and acceptor of BODIPY induced to separate electron distribution in HOMO and LUMO, induced singlet oxygen generation without bromine. To gain further insights into the results, The optimized structures, electron distributions of all the dyes were calculated, using the density functional theory(DFT) B3LYP/6-31G(d,p) level.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-372**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Mechanisms of CO₂ absorption and desorption of A₂CO₃-promoted MgO (A = Na, K, Rb and Cs))

Jin-Su Kwak, Kang Yeong Kim, Kyung-Ryul Oh, YOUNG UK KWON*

Department of Chemistry, Sungkyunkwan University, Korea

MgO is considered as a promising material for CO₂ absorbent in mid-term range (200 ~ 500 °C) because of low regeneration temperature of MgCO₃ into MgO and high theoretical absorption capacity. But, low reactivity with CO₂ is a major problem for application. In order to increase the reactivity with CO₂, alkali metal carbonates (A₂CO₃; A = Na, K, Rb and Cs) are known as a promoter for MgO. However, the promoting mechanism of alkali carbonate is not clearly proved. In this study, we clarify CO₂ absorption and desorption mechanisms of A₂CO₃-promoted MgO (A = Na, K, Rb and Cs). Before CO₂ absorption, absorbents were pre-treated in N₂ and this is key process for activating absorbent. During pre-treatment, A₂CO₃ is partially decomposed and A₂O is formed. A₂O is doped in MgO and it generates highly base sites on MgO surface. Depending on the A, absorbents show different CO₂ absorption and desorption properties. Heavier A₂CO₃-promoted MgO shows the fastest CO₂ absorption kinetics but their cycle is unstable. Detailed experiment data and their explanation will be presented in the poster session.

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Venue: Kimdaejung Convention Center, Gwangju

Code: MAT.P-373

Area: Material Chemistry

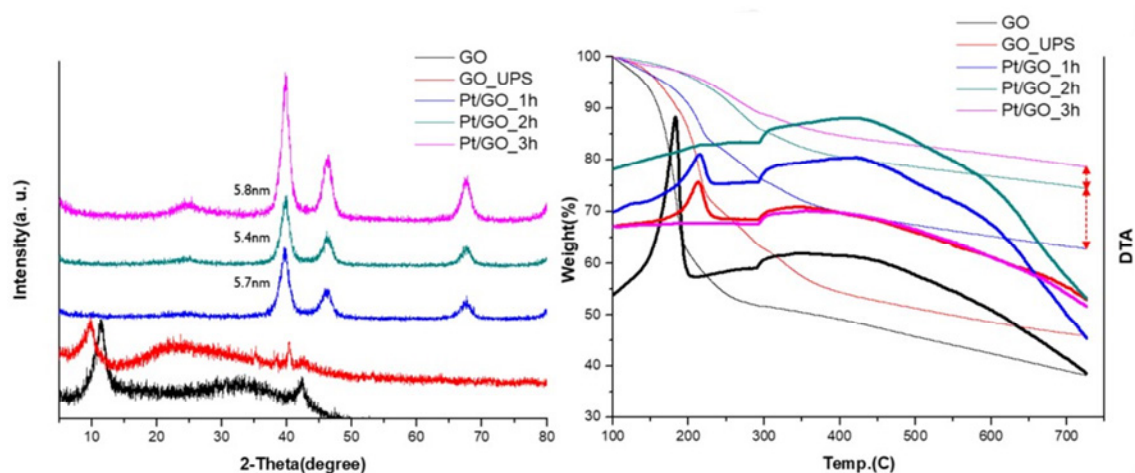
Type: Poster Presentation, Time: THU 11:00~12:30

Mechanism Study of Simultaneous Reduction of Graphene Oxide and Pt(II) through one-pot Ultrasound-assisted Polyol Synthesis (UPS)

Jongun Jung, Hyun-Uk Park, Ah Hyeon Park, WEN JUAN SHI, YOUNG UK KWON*

Department of Chemistry, Sungkyunkwan University, Korea

We report on the synthesis of reduced graphene oxide (RGO) supported Pt nanoparticles (NPs), in which was achieved via one-pot ultrasound-assisted polyol synthesis (UPS) reactions. Through the UPS mechanism, Pt(acac)₂ and graphene oxide (GO) were reduced simultaneously as Pt NPs and RGO, respectively. Based on observations from a series of control groups, we would like to propose a mechanism of the NPs' formation so called as seeding that enables control of the amount of reduced graphene oxide. Characterization of the composites by X-ray diffraction (XRD), thermogravimetric analysis (TGA) and differential thermal analysis (DTA) revealed reduction steps that platinum is first and graphene oxide is second. The Raman spectra of the Pt/RGO composites showed that a well reduction was happened during UPS. The merits of UPS simultaneous reduction in developing reduced graphene oxide supported composites are discussed.



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-374**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

On-chip silylation of nerve agents' degradation products for the head space GC-MS analysis using anion exchange polymeric film coated gold substrate

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Agency for Defense Development, Korea

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

Identification of alkyl methylphosphonic acids in aqueous samples is important for the monitoring compliance with Chemical Weapons Convention. In order to analyze the alkylmethylphosphonic acids in the complex matrices, it is essential to remove the interfering substance through a sample preparation process. In this study, we propose solid phase extraction of alkyl methylphosphonic acids using gold chips coated with poly(triethylammonium ethyloxymethacrylate) film prepared by surface initiated polymerization and the on-chip silylation of extracted alkyl methylphosphonic acids for Headspace GC-MS analysis. In this study, the proposed analytical method was optimized and verified through a series of experiments. The optimized method was successfully applied to OPCW proficiency test sample.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-375**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Gas Sorption on Nitrogen-doped Polar Carbons

JOO-WOON LEE

School of Liberal Arts and Sciences, Korea National University of Transportation, Korea

Templated carbons can have specific surface areas of 1500-1800 m²/g and average pore diameters of 2-11 nm. Nitrogen-doping these carbons modify their charge promoting their binding of ions and increasing thereby electrolyte permeation. Research presented here is the synthesis of a phase-pure crystalline precursor of a nitrogen-doped carbon, LaNTA·H₂O, where NTA is the tribasic nitrilotriacetate anion. Its pyrolysis at different temperatures followed by acid-extraction of the formed La₂O₃ yields nitrogen-doped templated carbons. They contain 1.4 to 7.9 atomic % of nitrogen at surface composition, the nitrogen content decreasing as pyrolysis temperature is increased. While the specific surface area increases from 330 to 1740 m²/g. Thermogravimetric analysis (TGA) is performed to determine gas adsorption-desorption characteristics of the nitrogen-doped carbons. These carbons initially adsorb 4 to 19 % of their weight from ambient room air (nitrogen, oxygen, moisture, etc.), and rapidly and reversibly ad/desorb dried air in TGA profile. The sorption capacity decreases as the pyrolysis temperature is increased. This was supported by Korea National University of Transportation in 2017.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-376**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of UiO-66-Type Metal–Organic Framework with Free Carboxylic Acid: Versatile Adsorbents via H-bond for liquid phase

JiYoon Song, Sung Hwa JHUNG*

Department of Chemistry, Kyungpook National University, Korea

MOFs with UiO-66 structure were synthesized from terephthalic acid (TPA), isophthalic acid (IPA) and zirconium chloride ($ZrCl_4$) to obtain free carboxylic acid on the MOFs. UiO-66 with free $-COOH$ can be obtained in a facile way by replacing up to 30% of the TPA with IPA. However, the chemical and thermal stability of the synthesized MOFs decreased with increasing IPA content used in the syntheses, suggesting an increase in the population of imperfect bonds in the MOFs because of the asymmetrical structure of IPA. The obtained MOFs with free $-COOH$ were applied in liquid-phase adsorptions from both water and model fuel to not only estimate the potential applications but also confirm the presence of $-COOH$ in the MOFs. The adsorbed amounts of several organics (triclosan and oxybenzone from water; indole and pyrrole from fuel) increased monotonously with increasing IPA content applied in MOF synthesis (or $-COOH$ in the MOFs). The favorable contribution of free $-COOH$ to adsorption can be explained by H-bonding, and the direction of H-bonds was confirmed by adsorption of oxybenzone in a wide pH range. The versatile applications of the MOFs with $-COOH$ in adsorptions from both polar and nonpolar phases are remarkable considering that hydrophobic and hydrophilic adsorbents are generally required for water and fuel purification, respectively. Finally, the presence of free $-COOH$ in the MOFs was confirmed by liquid-phase adsorptions together with general Fourier transform infrared analyses and decreased chemical and thermal stability. In summary, it was confirmed that UiO-66 with free $-COOH$ can be synthesized facily in one step from inexpensive IPA and TPA, and the obtained MOFs can be used in various adsorptions, especially in the liquid phase.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-377**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Removal of Pharmaceuticals and Personal Care Products from Water by Adsorption with Functionalized Metal-organic Frameworks: Contribution of Hydrogen-bonding

HyungJun An, Sung Hwa JHUNG*

Department of Chemistry, Kyungpook National University, Korea

Some pharmaceuticals and personal care products (PPCPs) (such as naproxen, ibuprofen and oxybenzone) were adsorbed from aqueous solutions on highly porous metal-organic framework (MOF) MIL-101 with and without functionalization. Adsorption results showed that MIL-101s with H-donor functional groups such as –OH and –NH₂ were very effective for naproxen adsorption, despite a decrease in porosity, probably because of H-bonding between O atoms on naproxen and H atoms on the adsorbent. For this reason, MIL-101 with two functional groups capable of H-bonding (MIL-101-(OH)₂) exhibited remarkable adsorption capacity based on adsorbent surface area. The favorable contributions of –OH and –(OH)₂ on MIL-101 in the increased adsorption of ibuprofen and oxybenzone (especially based on porosity) confirmed again the importance of H-bonding mechanism. The adsorbent with the highest adsorption capacity, MIL-101-OH, was very competitive when compared with carbonaceous materials, mesoporous materials, and pristine MIL-101. Moreover, the MIL-101-OH could be recycled several times by simply washing with ethanol, suggesting potential application in the adsorptive purification of water or removal of PPCPs.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-378**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Removal of Artificial Sweeteners from Water by Adsorption with Urea or Melamine-functionalized Metal-Organic Frameworks

DONGKYU YOO, Sung Hwa JHUNG*

Department of Chemistry, Kyungpook National University, Korea

Some N-containing compounds such as urea or melamine was introduced into a highly porous metal-organic framework (MOF), MIL-101, via grafting on open metal sites of the MOF. Adsorptive removal of three artificial sweeteners (ASWs) was studied using the MOFs, with or without modifications (including nitration), and activated carbon (AC). The adsorbed quantities (based on the weight of the adsorbent) of saccharin (SAC) under various conditions decreased in the order urea-MIL-101 > melamine-MIL-101 > MIL-101 > AC > O2N-MIL-101; however, the quantities based on unit surface area are in the order melamine-MIL-101 > urea-MIL-101 > MIL-101 > O2N-MIL-101. Similar ASWs [acesulfame (ACE) and cyclamate (CYC)] showed the same tendency. The mechanism for very favorable adsorption of SAC, ACE, and CYC over urea- and melamine-MIL-101 could be explained by H-bonding on the basis of the contents of -NH₂ groups on the MOFs and the adsorption results under a wide range of pH values. Moreover, the direction of H-bonding could be clearly defined (H acceptor: ASWs; H donor: MOFs). Based on their high adsorption capacity (for example, urea-MIL-101 had 2.3 times the SAC adsorption of AC) and ready regeneration, urea-MIL-101 and melamine-MIL-101 could be suggested as competitive adsorbents for removal of organic contaminants (such as ASWs) with electronegative atoms.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-379**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ni(II) Complex on Bispyridine-Based Porous Organic Polymer as Heterogeneous Catalyst for Selective Ethylene Dimerization

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Department of Chemistry, Korea University, Korea

A new porous organic polymer, POP-1 was synthesized through 'click reaction'-derived poly-triazole network between tetra(4-azidophenyl)methane (1) and 5,5'-diethynyl-2,2'-bipyridine (2). After treating with NiCl₂·(bpy)Ni(II)Cl₂-embedded porous organic polymer, Ni(II)-POP-1 was prepared. Brunauer–Emmett–Teller (BET) surface areas of POP-1 and Ni(II)-POP-1 shows 595 and 375 m²g⁻¹, respectively, as estimated by the N₂-adsorption isotherms at 77 K. Ni(II)-POP-1 was outstanding activities for the liquid-phase ethylene dimerization to selectively form 1-butene in the presence of Et₂-AlCl. Interestingly, Ni(II)-POP-1 shows higher catalytic activity than (bpy)Ni(II)Cl₂- homogeneous analogue under mild reaction condition (20 bar, rt). Ni(II)-POP-1 has a great potential application in ethylene dimerization, which is an important industrial process due to a high demand for alpha olefins.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-380**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Immobilization (bpy)Cu(II)Cl₂ into Stable Porous Organic Polymer Assembled by Co-Catalysed Trimerization and Its Oxidation of Various Olefins

Yi Jigyoung

Department of Chemistry, Korea University, Korea

We have developed a new class of porous organic polymer based heterogeneous catalyst Cu(II)-POP-1 based on the incorporation of (bpy)Cu(II)Cl₂ into porous organic polymer made of 5,5'-diethynyl-2,2'-bipyridine (1) and tetra(4-ethynylphenyl)methane (2) via cobalt-catalyzed acetylene trimerization. Cu was particularly interested due to its economical consideration. The use in heterogeneous catalysis for oxidation of various olefins has been successfully accomplished. Particularly, it showed good olefin oxidation activity compared to its homogeneous analogue, suggesting that the degradation of catalysts via the formation of less active aggregated species was successfully inhibited by successful site isolation via immobilization of catalysts on porous organic polymer support. Additionally, this heterogeneous catalyst shows good re-usability without losing their activity significantly.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-381**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of hollow nanostructured TiO₂/graphene hybrid for anodic material in sodium-ion battery

Won-Jae Lee, Seung-Min Paek^{*}

Department of Chemistry, Kyungpook National University, Korea

The titanium oxide (TiO₂) has considered as an anodic material in a rechargeable battery due to its structural and electrochemical stability. However, TiO₂ is hardly used in sodium ion battery because it has low electrical conductivity. Thus, in this study, the TiO₂/graphene hybrid with spherical hollow structure was synthesized via layer-by-layer self restacking by electrostatic interaction onto soft polymer template. According to the electron microscopic studies, the obtained TiO₂/graphene hollow spheres show that the products were formed with spherical hollow structure and their size was sub-micrometer. And in the energy dispersive spectroscopy results, the titanium and carbon atoms were homogeneously distributed in the final product. The FT-IR and Raman spectra show that the graphitic carbon was maintained in the TiO₂/graphene hollow sphere. In the electrochemical impedance spectroscopy, the obtained products have higher electrical conductivity than the bulk TiO₂. The half-cell tests for sodium ion battery show that the obtained TiO₂/graphene hollow sphere has higher specific capacity and better cycling performance at various current rates than those of the bulk TiO₂. The present TiO₂/graphene hollow sphere could be used as anodic materials for sodium ion batteries with enhanced performance.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-382**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ionic liquid@MIL-101(Cr) prepared via the ship-in-bottle technique: remarkable adsorbents for the removal of benzothiophene from liquid fuel

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Department of Chemistry, Kyungpook National University, Korea

Recently, there is a considerable demand to reduce the content of sulfur and nitrogen containing organic compounds in fuels like diesel and gasoline to a very low level to prevent air pollution and deactivation of catalysts. Metal-organic frameworks (MOFs) modified with the introduction of acidic ionic liquids (ILs) have been employed to the adsorptive removal of benzothiophene (BT) from n-octane. ILs were synthesized inside a porous MIL-101(Cr) via a ship-in-bottle (SIB) technique. The maximum adsorption capacities (Q_0) 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 Q_0 . The Q_0 value, based on the surface area (mg/m^2) 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 acid–base interactions between the acidic ILs and the slightly basic 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 over several cycles for adsorption of BT from liquid fuel.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-383**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Remarkable adsorption capacity of a Co-based metal azolate framework for removal of benzotriazole and benzimidazole from water

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Adsorptive removal of benzotriazole (BTA) and benzimidazole (BZI) using a Co-based metal azolate framework, MAF-5(Co), has been studied to understand the applicability of MAF in the removal of toxic water pollutant from contaminated water. The adsorption capacity of the MAF-5(Co) for BTA and BZI was highest than that of commercial activated carbon with other typical adsorbents including metal-organic frameworks (MOFs), even though the porosity of MAF-5(Co) was the lowest among the tested adsorbents. The remarkable adsorption of MAF-5(Co) was explained by hydrophobic effect and π - π interactions between the BTA and MAF-5(Co). Based on the zeta potential of MAF-5(Co) and effects of solution pH on the BTA adsorption, electrostatic interactions between the MAF-5(Co) and BTA species might also affect the adsorption of BTA over MAF-5(Co). Moreover, MAF-5(Co) can be regenerated by simple ethanol treatment and is reusable for adsorptive removal of BTA. Therefore, MAF-5(Co) can be suggested as a potential adsorbent for BTA and BZI removal from water based on their facile synthesis, highest adsorption capacity and excellent reusability. Keywords: adsorption; benzotriazole; benzimidazole; MAF-5(Co); water pollutant.

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Synthesis of Hydrophobic Cobalt-Ethylimidazolate Frameworks and Their Possible Application in Cleaning of Contaminated Water

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Phase-pure and high yield synthesis of two highly porous Co-based metal-azolate frameworks (MAFs), MAF-5(Co) and MAF-6(Co), which are isostructural with MAF-5(Zn) and MAF-6(Zn), respectively, were conducted at room temperature. Two mixing methods; slow and fast, were compared in the syntheses MAF-5(Co) and MAF-6(Co). The fast mixing of the reactant mixtures was found as the most effective for synthesizing MAF(Co) materials in pure-phase with high yield. The synthesized MAFs(Co) were found to be highly porous and very hydrophobic, similar to the MAFs composed of Zn, suggesting possible applications in water purification. To check the applicability, MAF-5(Co) and MAF-6(Co) were then applied to adsorb n-octane as a model oil and nonpolar adsorbate from water and the obtained results were compared to those of related materials, i.e., MAF-4(Co and Zn), MAF-5(Zn), and MAF-6(Zn), as well as with Cu-BTC (Cu-benzenetricarboxylate) and a conventional adsorbent, activated carbon. Surprisingly, even with low porosity, MAF-5(Co) showed remarkable competitiveness among the typical porous materials for n-octane removal. However, better performance of MAF-6(Co) was seen for the n-dodecane adsorption. The results suggest that the framework structure such as cavity and aperture sizes rather than surface area plays a significant role in the removal of hydrocarbon (n-octane or n-dodecane) from water. Moreover, MAF-5(Co) can easily be regenerated by simple evacuation and thus it can be suggested as a potential adsorbent for the removal of spilled oil from water. Additionally, the competitiveness of MAFs in the adsorption of diclofenac sodium from water, again suggesting as a good adsorbents in water purification probably because of hydrophobicity.

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Area: Material Chemistry

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Na storage behavior of Co₃O₄/graphene for electrochemical application

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The Co₃O₄/graphene composite was synthesized to used as an electrode material in secondary battery. The structure and physicochemical properties are characterized by XRD, SEM, TEM, FT-IR and RAMAN. The TEM image confirmed the Co₃O₄ nanoparticles were grown on the graphene nanosheets in the manner of covering the graphene surface and anchoring to the edge. In the electrochemical performance, the bare Co₃O₄ has poor rate capability and low capacity, which attributed to a volume variations and particle aggregation during the charge/discharge processes. However, by using graphene as a conductive support material, enhanced electrochemical properties such as improved electronic conductivity and fast ion diffusion were obtained. Graphene nanosheets in the product have a role as a buffer that alleviates volume changes, resulting in better stability and higher rate capabilities upon successive cycles.

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Type: Poster Presentation, Time: THU 11:00~12:30

Hyperbranched Polyglycerol-Grafted Graphene Oxide as a Reinforcing Material for Flexible Poly(vinyl chloride)

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We present a graphene oxide (GO) grafted with hyperbranched polyglycerol (HPG) as an effective reinforcing filler for flexible poly(vinyl chloride) (PVC). The HPG-grafted GO (HGO) is facilely synthesized by surface-initiated ring-opening polymerization of glycidol and followed by butyl esterification. The obtained HGO exists as an individually exfoliated nanosheet and possesses many functional groups, capable of interacting with PVC. Owing to the uniform dispersion of HGO and strong interfacial interactions between HGO and PVC, the PVC/HGO composites exhibit enhanced tensile strength and toughness compared with pristine PVC. In particular, the stretchability and ductility of PVC/HGO films are similar with the corresponding properties of pristine PVC film because the grafted HPG could act like a plasticizing agent at the interfaces. Furthermore, 2D planar structure and homogeneous dispersion of HGO provide high tortuous path to the composites, resulting in remarkably reduced oxygen permeability, more than 60% lower than that of pristine PVC only at low loading of HGO.

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GHz Band Selective Microwave Absorption Properties of Submicron Magnetite

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The increased development and use of electronic devices have led to a new kind of pollution known as electromagnetic interference(EMI). The interference effect leads to not only malfunction of electronic devices but also serious issues such as the human diseases like headache, leukemia and cancer. Many researchers have investigated the efficient shielding methods to reduce EMI. The aim of this work is to find out the effect of cluster size on the electromagnetic wave absorption properties. Investigation of these absorbers has mostly concentrated on the enhanced EM wave absorption performance. But the EM absorption material, which selectively shields frequency region is rarely reported. In this work, paramagnetic Fe₃O₄ nanoparticles are synthesized controlling the size of Fe₃O₄ nanoparticles by hydrothermal reaction. The X-ray diffraction patterns and scanning electron microscopy images have confirmed the formation Fe₃O₄ nanoparticles. We have studied the EMI shielding effect and EMI shielding mechanism of Fe₃O₄ nanoparticles of different sizes in the range of 1~18 GHz. The reflection loss shifted to the lower frequency with increasing thickness and also the reflection loss shifted to the lower frequency with increase in cluster size of Fe₃O₄ nanoparticles.

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Type: Poster Presentation, Time: THU 11:00~12:30

Enhanced Photofunctional Activity of ZnO Nanoparticles for UV-Vis Light Photodegradation

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Recently, with the growing demand for clean and comfortable environment, purification technologies with high efficiency and low cost are urgently in need. Thus for the remediation of hazardous wastes, many efforts have been taken in recent years by the use of ZnO catalyst for the photodegradation of toxic dye pollutants. ZnO having band gaps of 3.37eV at room temperature offers several advantages over other catalytic materials such as higher quantum efficiency, environmentally friendly, low cost and superior in photocatalytic activity. In this study, a facile and efficient approach for the fabrication of ZnO nanoparticles has been demonstrated. Microstructure and physical properties of the ZnO nanoparticles were investigated by field emission scanning microscopy (FE-SEM), transmission electron microscopy (TEM), infrared spectroscopy (IR) and steady state spectroscopic method. In addition, studies of the photocatalytic properties of the ZnO nanoparticles by exposure to UV irradiation of organic pollutants have demonstrated that they have potential photocatalytic applications.

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Type: Poster Presentation, Time: THU 11:00~12:30

A fluorescence carbon dot using nitrogen containing compound for bio imaging

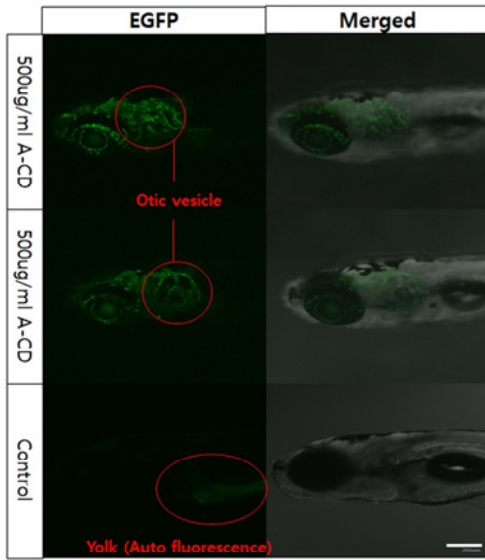
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We synthesized hydrothermally water-soluble A-CD(Alendronate-based carbon dots) using commercial osteoporosis medicine. Alendronate as the start material having Bisphosphonate group was used for osteoporosis treatment clinically and also are good candidates as a bone-imaging agent because of high affinity for Hydroxyapatite. A-CD were made from Bisphosphonate derivatives containing nitrogen compound as the source of carbon without surface passivation agent by hydrothermal method. We confirmed that they exhibited the highest fluorescence intensity at 405nm and good photo stability in DI-Water. Due to superior biocompatibility, A-CDs were imaging in living HeLa cells, which indicated that it is applicable in various fields of bio imaging. The high affinity of A-CD for hydroxyapatite also were verified through α -TCP(tri-calcium phosphate) scaffold incubated in A-CDs solution. As new fluorescent carbon material, advantages of A-CD include strong fluorescence, water solubility, unnecessary passivating agent, low cytotoxicity and high affinity for hydroxyapatite. These A-CD showed promising bone specific imaging due to their surface phosphonate-group and suitable candidates for the applications in the bio imaging field.



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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Detection of endocrine disruptors by M-13 virus-based structural color nanostructure

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Considerable social interest generated due to the side effects of endocrine disrupting chemicals. The structure of EDC, like benzene, mimics the mechanism of hormones occurring naturally in vivo and changes the physiology of the endocrine system. However, PCBs and phthalates in plastic products are still in use today, although representative EDCs such as PCBs(Polychlorinated Biphenyls) and phthalate compounds have already been banned in many countries. EDCs can be release from the product during use and/or disposal, and cause serious environmental problems. Here, we have developed a virus based on structurally colored nanostructures that are capable of sensitive and selective detection of even minute concentrations of EDC. These structurally colored nanostructures form a regular virus bundle structure through a simple pulling technique and exhibit a unique angle-independent color. By controlling the concentration of the virus solution and the pulling speed, this can create various color bands. Use M-13 bacteriophage genetically engineered to react with specific EDCs, PCBs and phthalates. The benzene derivative peptide was bound to the surface of M-13 bacteriophage(pVIII major coat protein) by phage library method. In the initial step, virus-based color sensor was exposed to a variety of organic chemicals. The sensitivity of the virus-based color sensor was tested along with the selectivity evaluation. 10 to 300 ppm of phthalic anhydride and chlorobenzene were detected by the color sensor and showed a remarkable sensitivity with a dissociation constant of about 90. All measurements were analyzed by Principal Component Analysis(PCA) and Linear Discriminant Analysis(LDA) and the notable point was a clear distinction when exposed to two categories of EDC(PCB and phthalate).

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Enhanced Electrocatalyst Performance of Mesoporous Carbon@Metal Oxide Heterolayered Hybrid Nanosheets

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Mesoporous carbon@metal oxide heterolayered hybrid nanosheets can be synthesized by the anchoring of mesoporous carbon on the surface of exfoliated metal oxide nanosheet. The exfoliated metal oxide acts as an efficient substrate for stabilizing two-dimensional lattice of mesoporous carbon with extremely high surface areas and controlled pore size distribution. Field emission-scanning electron microscopic and energy dispersive spectrometric analyses clearly demonstrate the formation of mesoporous carbon shell on the core of metal oxide 2D nanosheet. The resulting heterolayered hybrid nanosheets show outstanding electrocatalytic activity for oxygen reduction reaction with a lower on-set potential and a larger number of electron transfer (~4), which are much superior to that of mesoporous carbon. This is the first report about the heterolayered hybrid nanosheet of mesoporous carbon@layered metal oxide.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A Critical Role of 2D Metal Oxide Nanosheets as Additives for Improving the Electrocatalytic Performance of Graphene

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High performance Pt-free electrocatalyst can be synthesized by an addition of small amount of exfoliated metal oxide ($\text{CoO}_2/\text{Ti}_{1-x}\text{O}_2/\text{RuO}_2$) nanosheet into graphene suspension. The incorporation of metal oxide nanosheet is effective in increasing the surface area and pyridinic N content of N-doped graphene and also in decreasing its charge transfer resistance. Even at low content of metal oxide nanosheets (

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Area: Material Chemistry

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Development of anion adsorption material with calcium bentonite and quaternary alkyl ammonium

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Anion removal in water treatment is one of important issues because anion causes damage both human body and environment. Anion exchange resins of polymer base are widely used; however, anion exchange resins have disadvantages such as environmental problems of secondary waste, low performance by interference phenomena, and high cost. To overcome the disadvantages mentioned above, in this study, we developed an anion adsorption material for water treatment using calcium bentonite, an environmental friendly natural mineral, complexed with quaternary alkyl ammonium. In order to confirm the anion removal performance of the material, series of appropriate experiments to estimate adsorption equilibrium were carried out, and excellent performance of perchlorate removal was confirmed thermodynamically. Furthermore, adsorption properties were investigated with analysis equipments (i.e. SEM, EA, TGA, XRD, and FTIR) and computational approaches (i.e. molecular and adsorption modelling). By using calcium bentonite, which is an abundant resource, we suggested novel approach that how the disadvantages of the anion exchange resins used in conventional water treatment can be overcome. It is expected that the developed material could be applied to the water treatment process to be efficient.

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Type: Poster Presentation, Time: THU 11:00~12:30

Manganese Cobalt Nickel Oxide Nanosheet-based Photocatalyst for Efficient Visible-Light-Driven Hydrogen Evolution

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We are successful in synthesizing the nanohybrid of CdS-[Mn_{0.3}Co_{0.3}Ni_{0.3}]O₂ by an electrostatically-derived self-assembly between negatively-charged tertiary metal oxide nanosheets and positively-charged CdS quantum dots (QDs). In the obtained nanohybrids, the positively-charged CdS QDs with the particle size of ~2.5 nm are immobilized on the surface of negatively-charged [Mn_{0.3}Co_{0.3}Ni_{0.3}]O₂ nanosheets with the formation of mesoporous stacking structure. According to the diffuse reflectance UV-vis and photoluminescence spectroscopic analyses, the hybridization with [Mn_{0.3}Co_{0.3}Ni_{0.3}]O₂ nanosheet leads to the enhancement of visible light absorption and a strong electronic coupling between two components. The present CdS-[Mn_{0.3}Co_{0.3}Ni_{0.3}]O₂ nanohybrids exhibit higher photocatalytic performance for H₂ evolution under visible light irradiation than does CdS QD, which is attributable to the suppression of photoexcited electron-hole recombination, the enhancement of visible light harvesting ability, and the increase of electron mobility. This finding verifies the beneficial role of conductive [Mn_{0.3}Co_{0.3}Ni_{0.3}]O₂ nanosheet as a hybridization matrix in improving the photocatalytic activity of semiconducting materials.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ultra-Sensitive Bragg-Reflective Photoluminescent Porous Silicon for Explosive Vapors

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Novel photoluminescent Bragg-reflective porous silicon (PBR PS) exhibiting dual optical properties, both optical reflectivity and photoluminescence, were developed and used as explosive sensor. PBR PS samples were prepared by an electrochemical etch of n-type silicon under the illumination with a 300 W tungsten filament bulb for the duration of etch. The etching solution consisted of a 1:1 volume mixture of aqueous 48% hydrofluoric acid and absolute ethanol. Typical etch parameters for the generation of PBR PS involved using a periodic sine wave current with 10 repeats. PBR PS exhibits strong red color reflection at 650 nm and strong red photoluminescence at 650 nm. The optical properties of free-standing PBR PS were investigated. The front side surface of PBR PS shows both reflectivity and photoluminescence, however the back side surface of free-standing PBR PS shows only reflectivity without PL. Surface and cross-sectional morphology and optical characteristic were determined by using scanning electron microscopy and optical.

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Investigation on CO₂ Absorption of NaNO₃-promoted CdO at midtemperature ranges

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In this study, we explored the reaction system $\text{CdO(s)} + \text{CO}_2(\text{g}) \rightleftharpoons \text{CdCO}_3(\text{s})$ as a model system for CO₂ absorbent in the intermediate temperature range (300-400 °C). Pure CdO does not react with CO₂ at all up to 500 °C, but CdO mixed with an appropriate amount of NaNO₃ (optimal molar ratio NaNO₃/CdO = 0.14) greatly enhances the conversion of CdO into CdCO₃ up to about 80% (5.68 mmol/g). These NaNO₃-promoted CdO absorbents can undergo many cycles of absorption and desorption by temperature swing between 300 °C and 370 °C under a 100% CO₂ condition. Details of how NaNO₃ promotes the CO₂ absorption of CdO have been delineated through various techniques using thermogravimetry, coupled with X-ray diffraction and electron microscopy. Based on the observed data, we propose a mechanism of CO₂ absorption and desorption of NaNO₃-promoted CdO. The absorption proceeds through a sequence of events of CO₂ adsorption on the CdO surface covered by NaNO₃, dissolution of so-formed CdCO₃, and precipitation of CdCO₃ particles in the NaNO₃ medium. The desorption occurs through the decomposition of CdCO₃ in the dissolved state in the NaNO₃ medium where CdO nanoparticles are formed dispersed in the NaNO₃ medium. The CdO nanoparticles are aggregated into μm large particles with smooth surfaces and regular shapes.

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Area: Material Chemistry

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RuO₂ nanoparticles supported NaY zeolite for aerobic oxidation of benzyl alcohol: Effect of preparation methods on catalytic performances

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RuO₂ supported NaY zeolites were prepared via various pathways: (i) simultaneous crystallization of zeolite framework with RuCl₃ precursor (Ru(SC)/NaY), (ii) post ion-exchange with Ru(III) cations (Ru(IE)/NaY), and (iii) post support of preformed RuO₂ nanoparticles (Ru(PS)/NaY). X-ray diffraction analysis confirmed that RuO₂ phase was formed on the NaY zeolite. With TEM and CO chemisorption analyses, it was confirmed that the RuO₂ nanoparticles were supported inside or outside the zeolite crystals with uniform dispersion depending on the catalysts. The catalysts were tested in an aerobic oxidation of benzyl alcohol using molecular oxygen under ambient pressure condition at various temperatures. The results revealed that the catalytic performances involving turnover frequency (TOF), activation energy (E_a), rate constant and recyclability were remarkably changed depending on the catalysts. The Ru(PS)/NaY showed the highest TOF (33–48 h⁻¹), whereas the others gave much lower TOFs (9–12 h⁻¹). The Ru(PS)/NaY also had the highest E_a (48.39 kJ mol⁻¹), whereas the Ru(SC)/NaY and Ru(IE)/NaY had smaller E_a values (18.58 and 24.11 kJ mol⁻¹, respectively). Notably, the Ru(PS)/NaY gave remarkably higher pre-exponential factor of 5.22×10^5 h⁻¹, which is about 5 orders of magnitude larger than that of the Ru(SC)/NaY (7.15×10^0 h⁻¹). This suggests that collision between benzyl alcohol and molecular oxygen was very intensive on the Ru(PS)/NaY. The detailed results will be presented in this presentation.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of LTA Zeolites with Controlled Crystal Sizes for Selective Removal of Radioactive Ions

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LTA zeolites with various crystal sizes were synthesized by hydrothermal synthesis method, wherein various synthetic variables were carefully controlled. More specifically, effect of pH was investigated by controlling the relative ratio of tetramethylammonium hydroxide and sodium hydroxide in the synthesis gel composition. In addition, effects of aging time, synthesis time and hydrothermal temperature were also investigated profoundly. The resultant LTA zeolites were characterized with X-ray diffraction and scanning electron micrograph analyses. The results show that the variation of various synthesis parameters succeeded in the systematic control of crystal sizes between 75 nm to 2 μm with variation of size distribution. The series of LTA zeolites with controlled crystal sizes were ion-exchanged to Na^+ -form, which constructed LTA zeolites with aperture size of 4 Å. These zeolites were further investigated in the selective removal of radioactive ions such as Cs^+ and Sr^{2+} from the sea water. Depending on the crystal sizes of LTA zeolites, the adsorption kinetics and quantities were changed. The details of synthesis of LTA zeolites with controlled sizes and application in pollutant removal will be addressed in this presentation.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Monodisperse mesoporous silicon nanoparticles combined with sulfur-graphene oxide for efficient performance of lithium ion battery anode

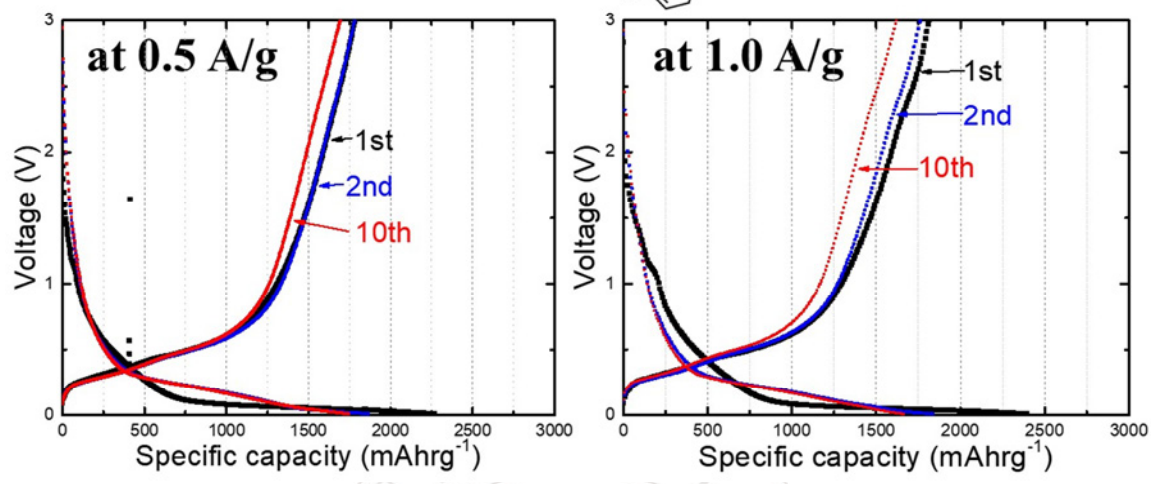
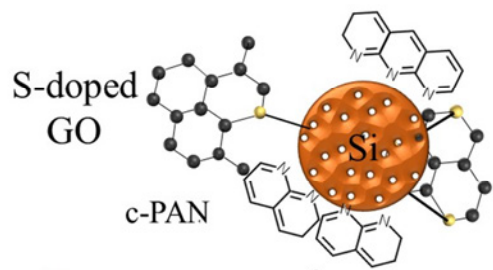
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Silicon nanoparticle is promising anode material for lithium-ion batteries(LIB) due to highest theoretical capacity (4200 mAhg⁻¹). However, instability issue during lithiation-delithiation and its low conductivity remain in the existing nanostructured silicon. To improve electrochemical stability, we synthesize Mesoporous silicon nanoparticle(mSiNP) by surface protected-magnesiothermic reduction. as-synthesized silicon combines Sulfur-doped graphene oxide with cyclized polyacrylonitrile(c-PAN) for enhance the electronic conductivity.



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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Preparation of electromagnetic shielding film based on carbon fiber reinforced with CNT

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A series of multi-walled carbon nanotube (MWCNT) coated carbon fabrics was fabricated with dip coating process, and their performance in thermal conductivity, thermal stability, tensile strength, electromagnetic interference shielding effectiveness (EMISE) was investigated. A solution of MWCNT oxide and sodium dodecyl sulfate (SDS) in water was used in the coating process. MWCNTs were observed to coat the surfaces of carbon fibers and to fill the pores in the carbon fabric. Electrical and thermal conductivities of the composites were 16.42 S/cm and 0.625 W/mK respectively. An EMI shielding effectiveness of 37 dB at 2 GHz was achieved with a single layer of coated carbon fiber fabric, whereas the double layers resulted in 68 dB EMI SE at 2.7 GHz.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Graphene coated non-woven carbon fiber based film for enhanced electromagnetic shielding effectiveness

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With a development of information technology and electronic devices, the importance of electromagnetic interference shielding has been increased. In this study, a series of graphene-oxide (GO) coated non-woven carbon fabric was developed, and their thermal, mechanical, electromagnetic interference shielding performance was inspected closely. Oxidation of Graphene was confirmed with XPS, XRD and Raman spectroscopy. Graphene oxide (GO) and polyvinylidene fluoride (PVDF) in N,N-dimethylformamide (DMF) solution was used in the coating process. PVDF filling the porous space between carbon fiber and GO substituted into PVDF matrix was observed.

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Phosphate adsorption behavior and luminescent property of layered yttrium hydroxide in aqueous solutions

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Excessive phosphorus (as phosphates in water) can cause serious eutrophication in lakes, reservoirs, rivers and oceans. On the other hand, phosphorus is essential nutrients for all living organisms, and applying to agriculture as fertilizer is important for food production. Given that only about 1/5 of phosphate fertilizers are included in the diet of humans and animals consumed by humans, most of them flow through food production and consumption. Therefore, special interest is needed to develop efficient materials that can recover phosphorus from environmental waters to reuse. In this study, we explored the possible applications of layered yttrium hydroxide *l*-Y(OH)₃ as an adsorbent for the phosphate recovery from water over a wide pH range. Compared to that (pH_{pzc} < 4) of hexagonal form *h*-Y(OH)₃, the surface charge of *l*-Y(OH)₃ is strongly positive up to pH ~ 11 (pH_{pzc} ~ 11). This new adsorbent revealed high capacity, efficiency, stability, selectivity, and reusability in adsorption of phosphate from a single electrolyte as well as natural waters containing competing anions. In particular, when Ce³⁺ and Tb³⁺ were co-doped (*l*-Y(OH)₃:Ce,Tb), phosphate adsorption led to the characteristic ⁵D₄ → ⁷F_J (J = 6, 5, and 4) emissions of Tb³⁺ under commercial 312 nm-UV irradiation. This “luminescence-on” behavior of *l*-Y(OH)₃:Ce,Tb by phosphate adsorption was employed to detect and recover phosphorus at low concentrations in deionized water, mineral water, tap water, and river water.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-403**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Inclusion behavior of bioactive anions into the interlayer space of LDHs vs. LRHs

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Bioactive compounds are very sensitive to light, temperature, and oxygen, etc., which limit their applications. Thus, it is desired if we can stabilize these molecules and protect them from rapid degradation by intercalating them into layered inorganic lattices. In this work, two families with typical 2-dimensional structure, layered double hydroxides (LDHs) and layered rare earth hydroxides (LRHs), were compared as host materials for common bioactive molecules. LDHs have attracted great interest due to their wide possible applications in diverse fields such as healthcare, drug delivery, food, cosmetics, etc. LRHs are structurally similar to LDHs and consist of positively charged rare-earth hydroxide layers with exchangeable, charge-balancing anions in the interlayer space. Due to the unique structure and properties, LRHs have also been recently investigated for applications as adsorbents, catalysts, drug carriers, and additives. The exchange capacity and arrange mode of anions in the interlayer galleries of LDHs and LRHs depends on the net positive charge of their hydroxide layers. The positive charge density of LDHs with general formula $M^{2+}_{1-x}M^{3+}_x(OH)_2A^{n-}_{x/n} \cdot mH_2O$ (A = interlayer anions) is controllable by adjusting M^{2+}/M^{3+} ratio, whereas LRHs with general formula $RE_2(OH)_5A^{n-}_{1/n} \cdot mH_2O$ (RE = rare earths) have a fixed charge density. Here, we demonstrate the similarity and difference in inclusion phenomena of common bioactive molecules, cinnamate, salicylate, ascorbate, tocopheryl acid succinate and citrate, in the interlayer space of LDHs and LRHs.

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Type: Poster Presentation, Time: THU 11:00~12:30

Silica coated CeO₂ particles with highly negative surface charge for UV screen

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Ceria (CeO₂) 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. Furthermore, when used as a coating material, ceria also displays effective corrosion protection properties. However, constructing composite coating films using ceria and inorganic species with accurate control in the coating structure has remained a challenge. In particular, layer-by-layer (LbL) deposition of alternating positive and negative layers require high difference in surface charge between layers. In this work, CeO₂ nanoparticles smaller than 20 nm in diameter were prepared for LbL deposition of UV-blocking multifunctional films. To enhance the negative surface charge, CeO₂ nanoparticles were coated with an amorphous silica (a-SiO₂), and their surface charge was highly improved to show the low point of zero charge ($\text{pH}_{\text{pzc}} < 3$). Thus, silica coated CeO₂ nanoparticles is very challenging as a negative UV-blocking layer material over a wide pH range, for LbL deposition with a positively charged inorganic species. These particles were well dispersed into water to form stable colloidal solutions that effectively screen UV.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Pt-Pd-Cu ternary alloy dendritic nanocrystals for enhanced electrocatalytic alcohol oxidation reactions

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Engineering the morphology and composition of multi-metallic nanocrystals composed of noble and 3d transition metals has been of great interest due to its high potential to the development of high-performance catalytic materials for energy and sustainability. In the present work, we developed a facile aqueous approach for the formation of homogeneous ternary alloy nanocrystals with a dendritic shape, Pt-Pd-Cu nanodendrites, of which synthesis has rarely been achieved due to synthetic difficulties. Proper choice of stabilizer and fine control over the amount of stabilizer and reductant allowed the successful formation of Pt-Pd-Cu nanodendrites. The prepared ternary alloy nanodendrites exhibited considerably improved electrocatalytic performance toward methanol and ethanol oxidation reactions compared to their binary alloy counterpart, Pt-Pd nanodendrites, and commercial Pt and Pd catalysts due to synergism between their morphological and compositional characteristics. We anticipate that the present approach will be helpful to develop efficient electrocatalysis systems for practical applications.

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Area: Material Chemistry

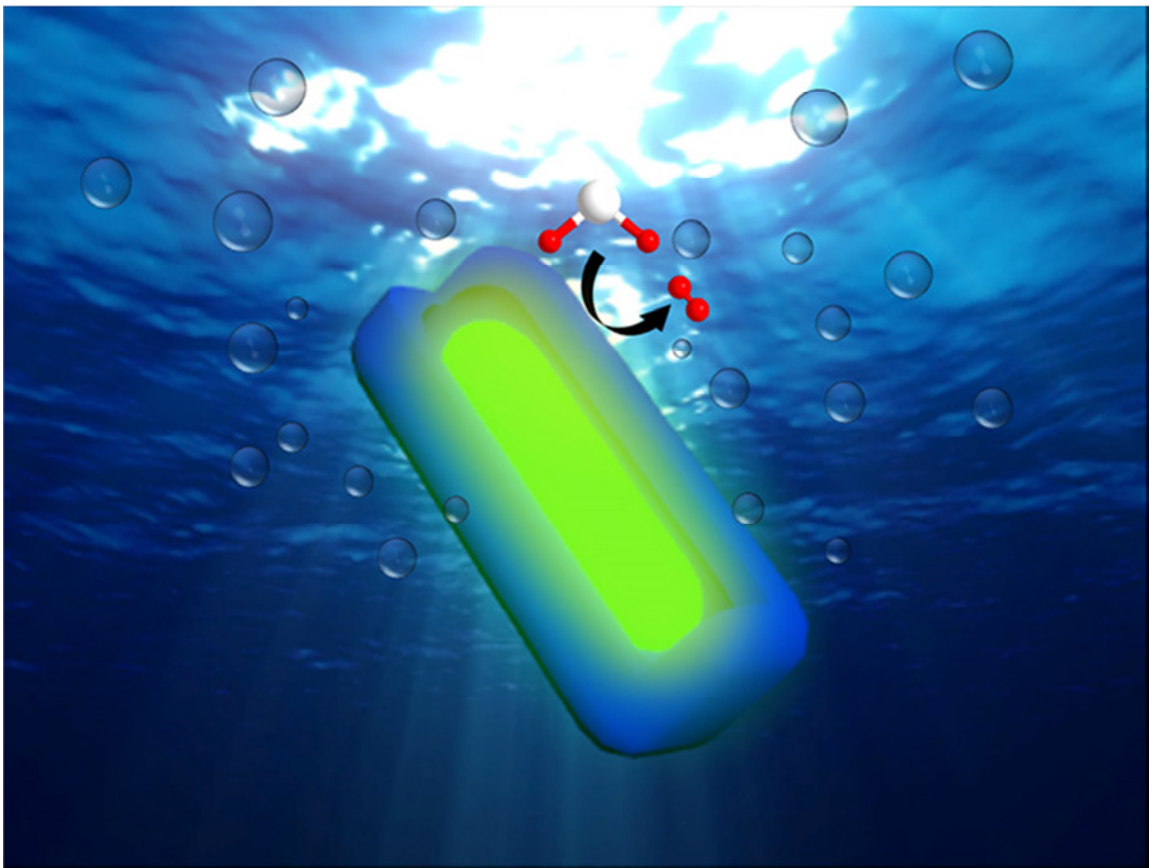
Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Au Nanorod-CdS Yolk-Shell Nanostructures and Their Enhanced Photocatalytic Hydrogen Evolution

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Plasmonic metal-semiconductor heteronanostructures with controlled topologies have attracted increasing attention as promising platforms for the efficient conversion of solar to chemical energy. Herein, we describe a novel synthesis route toward the formation of heteronanostructures with plasmonic metal yolks and semiconductor shells, which can enable the elevation of light harvesting efficacy. Au nanorod-CdS yolk-shell nanostructures with well-defined structural configurations were realized by a sulfidation and a subsequent cation exchange reaction with pre-synthesized Au nanorod@Ag core-shell nanostructures. The prepared yolk-shell nanostructures showed superior photocatalytic hydrogen evolution performance under visible light irradiation over their core-shell nanostructure counterparts, CdS hollow nanoparticles, and Au nanorods. A series of mechanistic studies on the photocatalysis distinctly corroborated that the pronounced photocatalytic function of the yolk-shell nanostructures is due to the synergism between the radiative relaxation of the plasmon energy of the Au nanorod yolks and the multiple reflections of the incident light within their voids rendered by the yolk-shell structure, which can promote the light absorption of CdS that can drive the photocatalysis. This study can provide a new perspective for designing hetero-nanoarchitectures with intended structures and desired functions.



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Photocatalytic effect of $\text{Fe}_3\text{O}_4@\text{TiO}_2$ enhanced by noble metals

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Tar pigment in azo dyes, widely used in the printing and textile industries, are harmful organic substances that cause human health problems. Recently, rapid removal and decomposition techniques of organic pollutants are required and studied. The photocatalysts, $\text{Fe}_3\text{O}_4@\text{TiO}_2$, and $\text{Fe}_3\text{O}_4@\text{TiO}_2\text{-M}$ (M=Ag, Au), used in this experiment were confirmed to be synthesized through field emission-scanning electron microscope (FE-SEM), X-ray diffractometer (XRD), fourier transform infrared spectroscopy (FT-IR) before photocatalytic experiments. In photodegradation experiments, the photocatalytic activity of the organic dyes Rh.B, 2,4,6-TCP and MP was gradually improved in the order of Fe_3O_4 , $\text{Fe}_3\text{O}_4@\text{TiO}_2$, $\text{Fe}_3\text{O}_4@\text{TiO}_2\text{-Ag}$ and $\text{Fe}_3\text{O}_4@\text{TiO}_2\text{-Au}$. Therefore, in this experiment it was confirmed that the catalytic effect is improved through visible light by accumulating TiO_2 and the noble metals on surface of the Fe_3O_4 core. Finally, the reuse analysis was performed five times for commercial purposes. It has confirmed that the photocatalytic efficiency did not reduce after 5 times of reuse.

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Code: **MAT.P-408**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and Crystal Structure of the New Two-dimensional Mixed-Metal Thiophosphates, $A_yTa_{(1-x)}Ti_xPS_5$ (A = K, Rb, Cs)

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The new two-dimensional mixed-metal thiophosphates, $A_yTa_{(1-x)}Ti_xPS_5$ (A = K, Rb, Cs), have been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. The title compounds crystallize in the space group $Fddd$ (A = K, Rb) and $P2_1/n$ (A = Cs). The statistically disordered Ta/Ti atoms are surrounded by six sulphur atoms in the distorted octahedral fashion and phosphorus atoms are coordinated by four sulphur atoms in a tetrahedral geometry. The two octahedral are combined to form $(Ta/Ti)_2S_{10}$ dimer and these dimers are connected through PS_4 tetrahedra to build the two-dimensional infinite anionic layers, $^{2-}_\infty[Ta_{(1-x)}Ti_xPS_5^y]$. Alkali metal ions reside among the layers to complete the three-dimensional structures. The classical charge valence can be described as $[A^+]_y[Ta^{5+}]_{(1-x)}[Ti^{4+}]_x[P^{5+}][S^{2-}]_5$.

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Code: **MAT.P-409**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Correlation between emitter orientations and molecular structures in TADF-based OLEDs

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In small molecule organic light-emitting diodes (OLEDs) which are implemented with emitters doped in host materials, the emitters' orientation is known to be very important for improving the out-coupling efficiency. In comparison with the internal quantum efficiency which has reached almost 100% such as using a thermally activated delayed fluorescence (TADF), a light out-coupling efficiency still has room to be enhanced. To control the orientation of emitter molecules in a host matrix, understanding of the molecular properties of dopant and host molecules and their interactions is required. However, the intrinsic molecular characteristics for horizontal orientation are not well-known especially for host molecules. In this work, we utilized angle-dependent photoluminescence (PL) measurements combined with quantum chemical calculations to investigate the orientations of several dopant molecules doped in different types of host molecules. Our experimental and computational results demonstrated that the linear and planar dopant molecules prefer horizontal orientation in our host materials. Moreover, at a low doping concentration (15 ± 1 wt. %), the strong interactions between host and dopant molecules can lead to the horizontal orientation of dopant molecules. Our donor-acceptor-donor typed hosts with tilted structures are found to interact strongly with dopant molecules due to their localized electron density. Consequently, our current results can provide design strategies for emitting layer molecules to develop highly efficient TADF OLEDs.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-410**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Magnetite Halloysite Nanotube and its Application for the Removal of Heavy Metals

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A unique nanostructured magnesium oxide coated magnetite clay composite was synthesized by a simple method using chemicals such as iron(II) sulfate heptahydrate ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$), magnesium(II) nitrate hexahydrate [$\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$], tetraethyl orthosilicate (TEOS), and urea. A new type of magnetic halloysite nanotubes (M-HNT) was characterized using X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), and Fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), and ultraviolet-visible spectroscopy. The halloysite nanotubes (HNT) were functionalized by the carboxyl group to control aggregation and stabilization. HNT-COOH can be easily collected and separated by adjusting the solution pH without additional filtration, sonication, or centrifugation. By changing the solution pH, HNT-COOH was easily dispersed, and the aggregation process was reversible. M-HNT-COOH had excellent removal capacities towards a specific heavy metal. (Cr(VI), Cu(II)) and the adsorption capacities were as high as 312 mg g^{-1} for Cu(II), 79 mg g^{-1} for Cr(VI). In this study, we demonstrated that M-HNT-COOH nanocomposites can be used for the removal of heavy metals from waste water and can be reusable by a simple and fast magnetic separation.

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Code: **MAT.P-411**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Phenolic Polymer Developers for Thermal Papers: Synthesis, Characterization and Developing Property

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Recently the demand for a safer alternative to bisphenol A (BPA, 4,4'-(propane-2,2-diyl)diphenol)-based developer materials for thermal (printing) papers has grown considerably because of the many potential health effects of exposure to BPA. In this study, in order to replace a problematic BPA developer for thermal papers, phenolic polymers were synthesized and their chemical structures were characterized by ¹H-NMR, FT-IR and GPC measurements. The thermal properties and color-forming reaction properties of these polymers were investigated in detail. In addition, the developing capabilities of the thermal papers using these phenolic polymers as developers were assessed and compared to those of BPA thermal papers.

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Code: **MAT.P-412**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Transition Metal diethyldithiocarbamate for solution synthesis of CIGS thin film photovoltaic cells

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Precursors of Cu, In, Ga diethyldithiocarbamate(ddtc) were prepared and deposited on glass substrate by spin coating method for fabrication of CIGS thin film. Cu, In and Ga ddtc compounds were synthesized separately by using CuCl_2 , InCl_3 , $\text{Ga}(\text{NO}_3)_3$ and Naddtc in aqueous solution. The crystallinity of these precursors was confirmed by XRD and coordination between metal and ligand was observed by FT-IR measurements. Dichloromethane was used to solve these compounds and black solution was obtained. The thin film was prepared by spin coating. Precursors on the film vaporized after annealing at 200°C , so we chose another method to observe synthesis of CIGS thin film. The mixture of solid phase as ratio (Cu:In:Ga) 3:2:1 was deposited on glass substrate at 450°C . Each thin film was measured by SEM and EDS to analyze thickness and chemical composition. TGA was utilized to analyze melting point of precursors and mixture of all precursors to investigate the optimal reaction condition for synthesis of CIGS thin films of photovoltaic cells.

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Code: **MAT.P-413**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Two-Dimensional Structure of Germanium Arsenide

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The increasing energy demand and the environmental issues caused by fossil fuels have led to the intense search for clean energy. Hydrogen is considered the ideal sustainable alternative to fossil fuels. Photoelectrochemical(PEC) water splitting for hydrogen generation has been attractive as it can store solar energy in the form of hydrogen. The recent discovery of graphene has given rise to significant interest in searching for new two-dimensional (2D) materials with their three-dimensional prototypes, where the 2D layers are stacked with weak van der Waals interactions. One of remarkable properties of the 2D nanostructures is their unique quantum confinement effect at the 2D limit. In the present work, we synthesized the germanium arsenide nanosheets using the exfoliation of bulk crystals that were synthesized by Bridgeman melt-growth method. Bulk GeAs is found to have a band gap (E_g) of ~ 1 eV, while the GeAs monolayer has been predicted to have $E_g = 2.1$ eV. We fabricated the Si/GeAs core/shell nanowire array that acts as a photoelectrode in the solar-driven water-splitting reaction, and observed the higher photocurrent with decreasing the layer thickness.

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Code: **MAT.P-414**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nickel carbide with N-doped CNT as bifunctional catalyst for oxygen reaction

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Development of high-performance catalysts is very crucial for the commercialization of sustainable energy conversion technologies. Efficient bifunctional catalysts for electrochemical oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are highly desirable due to their wide applications in fuel cells and rechargeable metal air batteries. However, the development of nonprecious metal catalysts with comparable activities to noble metals is still challenging. As a potential alternative to such catalysts, this investigation addresses the facile synthesis of an efficient and durable NiC@CNT hybrid bifunctional electro-catalyst for ORR and OER compared to commercial Pt/C catalyst. Crucially, this approach is green, facile, catalyst-free, and especially can be operated under ambient environments. Our works may expand the scope of cost-effective electrocatalysts for oxygen reaction.

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Code: **MAT.P-415**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

IrO₂ -ZnO hybrid nanoparticles for highly selective CO₂ reduction reaction

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The rising atmospheric concentrations of greenhouse gases, especially CO₂, are among the most pressing social issues today. The electrochemical CO₂ reduction reaction (CO₂ RR) is a key reaction for CO₂ conversion to valuable fuels and chemicals. Metals, such as Cu, Ag, Au, and Zn, are typical catalysts to reduce electrochemically CO₂ to the molecules in aqueous electrolytes. Development of low-cost high-performance catalysts is very crucial for the commercialization of CO₂ RR technologies. Here, we report a low-cost high-efficiency catalyst, iridium oxide -zinc oxide (IrO₂-ZnO) hybrid nanoparticles, which exhibit 80 % Faradaic efficiency of CO₂ reduction to CO at -1.0 V versus RHE. In order to understand the remarkable catalytic efficiency of IrO₂-ZnO, the electronic structures were thoroughly investigated using synchrotron X-ray photoelectron spectroscopy in combination with various electrochemical analyses.

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Code: **MAT.P-416**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Co-catalyst Modified Si-based Photo electrode Materials for Solar Water Splitting

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Photoelectrochemical (PEC) water splitting is a highly controlled approach that converts sunlight into clean, preserved hydrogen and oxygen. Photoelectrode consists mainly of two parts: light absorber and other is the cocatalyst. Si, having band gap of 1.1 eV poses suitable band alignment for H₂ evolution. Being the earth abundant semiconductor it is explored as an efficient light absorber material from past. However, stability and slow surface reactions limit the actual application of the material. Other important part in PEC cell is suitable cocatalyst, which helps in faster charge carrier transportation from semiconductor surface to electrolyte. In this regards, NiSe₂ and CoSe₂ are getting explored as efficient and stable material. In the present work, we developed CoSe₂ and NiSe₂ coupled with a Si nanowire array that acts as a promising bifunctional photoelectrode in the solar-driven water-splitting reaction.

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Code: **MAT.P-417**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Organic molecule-intercalated MoS₂ nanosheets for highly active hydrogen evolution reaction

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Hydrogen generated from water splitting has great potential for use as a clean, recyclable, and relatively low-cost energy source. Currently, Pt is state-of-art catalyst as only small overpotentials are required for high reaction rates. However, the scarcity and high cost of Pt limit its widespread technological use. This limitation has motivated significant efforts toward replacing Pt with earth-abundant non-noble metal materials. Transition metal carbides are one type of attractive materials, which exhibit good stability in acidic and basic media compared to their pure metal counterparts. Motivated by the novel properties of two-dimensional materials, MoS₂ has been extensively explored with discoveries surging in the recent years. Such impressive progress benefits from the success in synthesizing nanostructured MoS₂ in large scale. Herein, we report one-step hydrothermal synthesis of MoS₂ nanosheets using dimethyl-p-phenylenediamine (DMPD) as guest molecule. The MoS₂ nanosheets possess remarkably expanded interlayer spacing (1.0-1.3 nm), and the controlled phase (semiconducting 2H and metallic 1T) by the intercalation of DMPD. As the concentration of DMPD and/or the sulfur vacancies increases, they prefer to have the 1T phase with excellent catalytic performance for hydrogen evolution reaction. First-principle calculation predicted that the 1T phase MoS₂ becomes favorable by increasing the S vacancies and DMPD. The present work challenges the control of the electronic structures of MoS₂ nanosheets by intercalating the electron donating molecules.

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Facile Ultrasound Synthesis of Composition- and Size- Controlled Lead Halide Perovskite Nanocrystals

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Lead halide perovskites APbX_3 have attracted enormous interest as excellent light absorber material in photovoltaics with the power conversion efficiency exceeding 20% owing to their excellent optical and optoelectronic properties. Among the perovskite exhibit remarkable properties, thermal and air stability are critical for application. Herein, we report a novel ultrasound-induced synthesis method that can be applicable for wide-range composition A_4PbX_6 perovskite, where $\text{A} = \text{CH}_3\text{NH}_3$ or Cs and $\text{X} = \text{Cl}$ or Br , I . So called Zero-dimensional perovskite, A_4PbX_6 perovskite NCs are new frontier of perovskite-based materials show distinctive optical properties. Ultrasonic irradiation accelerates the dissolution of precursors in toluene, which determines the growth rate of NCs. It serves as a practical method to achieve monodisperse A_4PbX_6 , broadening the library of metal-halide perovskite nanomaterials.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Arsenic and Germanium Arsenide for High-Capacity Lithium Ion Batteries

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We report arsenic (As) and germanium arsenic (GeAs) as a promising alternative to commercial carbon materials in lithium ion batteries (LIBs). The As (or GeAs) and carbon (C) hybrid nanocomposites were synthesized using a ball-milling method. We first synthesized GeAs nanosheets by a liquid exfoliation of bulk crystals that were synthesized by Bridgeman melt-growth method. The electrochemical properties of As/carbon and GeAs/carbon hybrid nanocomposite for LIBs were investigated using an experimental and theoretical approach. The LIBs showed excellent cycling performance, with a reversible capacity of 1400 mA h g⁻¹ (after 100 cycles). Extensive first-principles calculations were performed employing a structure prediction method for crystalline Li_xAs (x = 1–6) phases, as well as ab initio molecular dynamics simulations for their amorphous phases. The capacity increase after repeated cycles is explained by a progressive amorphization, since the amorphous phase holds a larger capacity than the crystalline phase. Comparisons of the theoretical discharge curves with the experimental data provide valuable information for the development of high-performance LIBs.

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Area: Material Chemistry

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Composition Tuned $(\text{GaAs})_{1-x}(\text{Ga}_2\text{Se}_3)_x$ Ternary Alloy Nanowires

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Multicomponent nanowires (NWs) are of great interest for integrated nanoscale optoelectronic devices owing to their widely tunable band gaps. In this study, we synthesize a series of $(\text{GaAs})_{1-x}(\text{Ga}_2\text{Se}_3)_x$ ternary composition alloy nanowires using the vapor transport method. The formation of a cubic (zinc blende) phase solid solution at the composition range of $x = 0 - 1$ allowed the tuning of the band gap (1.4–2.0 eV). Pure GaAs NWs were synthesized with [111] growth direction using a hydrogen gas flow during the growth. As the Ga_2Se_3 incorporated during the growth under H_2 flow, the NW becomes defect-free single-crystalline and their growth direction is converted homogeneously into [110]. The Ga vacancies of Ga_2Se_3 along the [110] direction may also contribute to produce the uniform growth direction of NW. The incorporation of Se into the GaAs nanowires induces higher photo-sensitivity and lower dark current, which opens up a new strategy for enhancing the performance of photodetectors.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Metal Nanoparticle-Deposited ZnO Nanowires for Electrochemical and Photoelectrochemical Reduction of CO₂

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Reduction of CO₂ has been receiving increasingly considerable interest in terms of environmental and long-term energy security. Here, we report that ZnO nanowire array deposited with metal-nanoparticles (Au, Ag, Pt) was synthesized as efficient electrocatalysts and photoelectrocatalysts for CO₂ reduction reaction. Vertically aligned ZnO nanowires were synthesized by the chemical vapor deposition (CVD) on indium tin oxide (ITO) substrates. A successive ion layer adsorption (SILAR) method was developed to deposit the metal nanoparticles. We proposed that these nanowire array are credited to a synergic effect of excellent efficiency and high selectivity of CO₂ reduction to CO. This finding may lead to a new strategy for developing cost-effective electrocatalysts and photoelectrocatalysts for reducing CO₂.

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Visualized Lattice Mismatch of Polytypic GaP and GaAs Nanowires by Strain Mapping

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Zinc blende (ZB) phase group III-V semiconductor nanowires (NWs) often contain the polytypic structures owing to the existence of hexagonal phase. Therefore, characterization of polytypic structures is of great importance for various promising applications. In the present work, we synthesized various polytypic GaP and GaAs NWs with a controlled growth direction ([111] and [211]) using the chemical vapor transport method. Micro-Raman spectrum collected for individual NWs identified the E_2^H mode peak, which support the portion of hexagonal phase in the polytypic structures. Strain mapping of the NWs was obtained using the nanobeam precession electron diffraction technique. It visualizes remarkably the lattice expansion of the polytypic structures along the [111] direction, which can exceed 1%. This lattice expansion would originate from the larger lattice constant (c) of hexagonal phase than that of ZB phase. We fabricated the photodetectors using individual NW, showing the depression effects of polytypic structures on the photosensitivity. Our work provides new insight into the polytypic NWs, which is of paramount importance in the performance of nanoelectronics.

Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: **MAT.P-423**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Stable 1T phase MoS₂ nanosheets as Catalysts for Hydrogen Evolution Reaction

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Most recently, much attention has been devoted to 1T phase MoS₂ because of its distinctive phase-engineering nature and promising applications in catalysts, electronics, and energy storage devices. Herein, we report for the first time a simple one-step hydrothermal synthesis of the 1T phase MoS₂ nanosheets that are intercalated with methyl ammonium (MA). The nanosheets exhibit considerably expanded interlayer spacing as large as 9.6 nm with an 56% expansion as compared to that (0.615 nm) of the bulk counterpart. For comparison, we synthesized ammonium-intercalated MoS₂, which provides robust evidence for the stable 1T phase of these MA-intercalated structures. Their excellent electrocatalytic HER performance is demonstrated, suggesting a promising way to design advanced HER catalysts through modulating the phase and the interlayer distance. We performed first-principle calculation to obtain the intercalation energy of the 1T phase MA-intercalated MoS₂ nanosheets, which is more stable than the case of NH₄.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-424**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Chemical Compositions of Essential Oils Extracted from Citron Seed by Supercritical Carbon Dioxide

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This study was carried out to investigate the chemical composition of citrus seed essential oil extracted by supercritical carbon dioxide. The extract was analyzed by GC and GC-MS technique. The extraction of essential oil using in a semi-continuous flow extractor at the range of pressure and temperatures 150 to 400 bar and 30 to 50°C, respectively. The extraction condition for maximum yield was determined with the extraction yield of 22.1 wt% at 40°C of temperature and 280bar of pressure. The citrus seed essential oil was composed of five major components in the order of linoleic acid, oleic acid, palmitic acid, stearic acid and linolenic acid. Limonene was analyzed as the major volatile component of citrus seed essential oil.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-425**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

KVP₂O₇ as a Robust High-Energy Cathode for Potassium-Ion Batteries: Pinpointed by a Full -Screening of Inorganic Registry under a Specific Search condition

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Department of Printed Electronics Engineering, Suncheon National University, Korea

We data-mine the ICSD to find out the promising cathode materials for potassium ion battery (KIB). This is carried out to sequentially screen out the compounds that do not meet certain criteria. We further narrow down the promising candidates by predicting the properties through a density-functional-theory (DFT) and examining electrochemical properties experimentally. The pin-pointed compound KVP₂O₇ is thoroughly investigated. A superior energy density, rate performance, and stability are proved. In addition, its phase-transition behavior during charge-discharge (C-D) is also investigated. The galvanostatic C-D at various current densities revealed that the maximal capacity could be obtained at 0.25C. The changes of the 1st C-D profiles when the current densities were decreased from 0.25 to 10.0C at 50 °C. As expected, the increase of a current density induced the increase of overpotentials, which limited the high-potential redox process. The high-potential discharge capacity was continuously reduced with a current density, which led to a reversible capacity of 37 mAh·g⁻¹ at 10.0C. Despite the reduction in the discharge capacity and the average potential with a current density, however, the characteristic of high energy density of KVP₂O₇ was maintained. The ED of 253 Wh·kg⁻¹ at 0.25C was decreased to 146 Wh·kg⁻¹ at 10.0C, indicating that the 58 % energy still was utilizable even after the increase of a current density by 40 times. Furthermore, the ED of 253 Wh·kg⁻¹ was the highest value ever reported. The Ragone plot of KVP₂O₇ clearly demonstrates the retention of high ED with a change of power densities from 100 to 4000 W·kg⁻¹.

¹.*Keywords: data-mine, potassium ion battery, cathode, high energy density.*

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-426**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Mixed Metal Quaternary Spinel Type Compounds and Their Physical Properties

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Spinel-type lithium manganese oxides have received considerable attention as Li^+ ion selective adsorbents. Among them, quaternary mixed metal spinel compounds are expected to have the optimized structure for the Li^+ selective adsorbents because of their relatively low dissolution ratios of metal ions in the framework and good Li^+ adsorption capacity. In this study, we have prepared homogeneous $\text{LiM}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ($\text{M}=\text{Co}, \text{Fe}, \text{Ni}$) with various morphologies. Their Li^+ adsorption capacities and specific surface areas are measured and compared to find out any correlation between the Li^+ adsorption capacities and their physical properties. The characterization of $\text{LiM}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ($\text{M}=\text{Co}, \text{Fe}, \text{Ni}$) is performed by X-ray powder diffraction (XRD), inductively coupled plasma-atomic emission spectroscopy (ICP-AES), BET method, and scanning electron microscope (SEM).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-427**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Correlation between structure and luminescence property of copper halide complexes

**JuHyun Kim, Jaegyom Kim, Ha Eun Lee, dohee park, Woojin Yoon, Seung-Joo Kim^{*},
Hoseop Yun^{*}**

Department of Energy Systems Research, Ajou University, Korea

It is known that copper(I) halide complexes exhibit various structures and show different optical properties according to their structures. In this study, new copper halide complexes were synthesized by using various amine-based organic ligands: e. g. monoethanolamine (mea) and melamine, respectively. Single crystals of the compounds were grown employing the solvothermal method. Their crystal structures were determined by single crystal X-ray diffraction. The structure of $\text{Cu}_4\text{I}_4(\text{mea})_4$ are built-up from a cubane-like tetramer, which has an orthorhombic symmetry. $(\text{CuX})\text{melamine}$ ($X = \text{Br}, \text{I}$) consists of a stair step $(\text{CuX})_n$ polymer, which has a triclinic symmetry. The maximum excitation-emission wavelengths in the photoluminescence spectra were varied on the ligands in both structures. The relation between the crystal structure and the photoluminescence property will be discussed.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-428**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Na_xCrO_2 as promising intercalation host for potassium ion batteries

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Radical expansion of portable electronics over the decade has led to the intense exploration and exploitation of Li ion based battery (LIB) materials. Acute depletion of Li ion raw materials and surge in its manufacturing cost has driven the researchers towards other mono, di and tri-valent ion based secondary batteries. Among them, potassium ion batteries is promising for its close standard reduction potential (-2.9 V vs SHE) with lithium (-3.0 V vs SHE) and relatively low cost. Owing to the success of LiCoO_2 for LIB's, to start with, potassium based layered transition metal oxides would be the obvious choice. Previously, K_xCoO_2 and K_xMnO_2 were found to be active for reversible potassium (de)intercalation delivering a maximum specific capacity of 60 and 65 mAhg^{-1} respectively. Here, we have utilized O3-type NaCrO_2 that is revered as a high rate and extremely safe cathode material for sodium ion batteries (SIB's) to be an intercalation host for potassium ions. A cell constructed using NaCrO_2 as cathode, K-metal anode and 0.5 M KPF_6 as electrolyte delivered a reversible capacity of 72 mAhg^{-1} at C/20 current rate. Voltage profile depicted several potential steps in steep contrast to bi-phasic plateaus observed for the case of SIB's, reflecting successful K^+ intercalation into the Na_xCrO_2 host structure rather than Na^+ . Further, X-ray diffraction studies conducted on the cycled electrode revealed the co-existence of potassium rich- K_xCrO_2 and sodium rich Na_xCrO_2 phases suggesting a reversible (de)intercalation of K^+ ions into the host structure. The material also exhibited good rate capability by delivering a specific capacity of 52 mAhg^{-1} at 1C rate retaining nearly 72% of its initial capacity (C/20).

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Code: **MAT.P-429**

Area: Material Chemistry

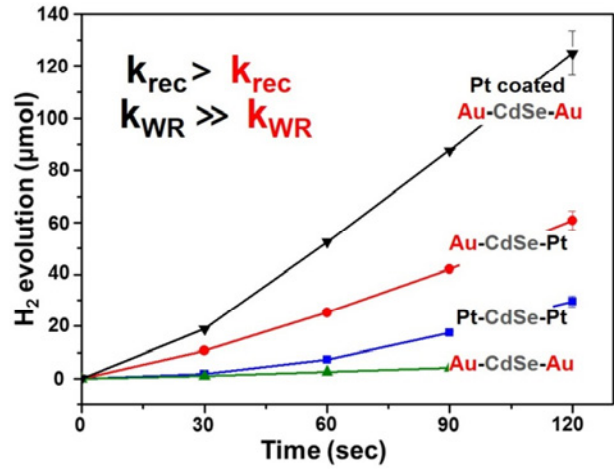
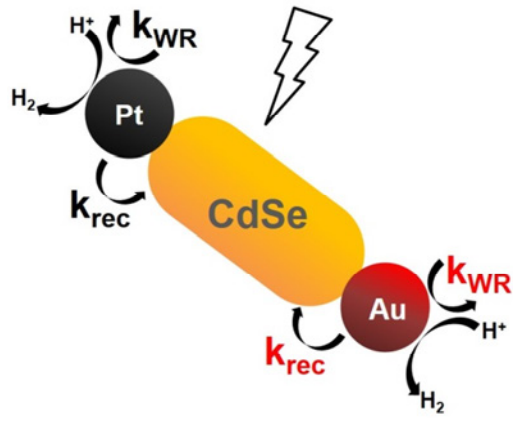
Type: Poster Presentation, Time: THU 11:00~12:30

Engineering Reaction Kinetics by Tailoring the Metal Tips of Metal-Semiconductor Nanodumbbells

JiYong Choi, Hyunjoon Song*

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Semiconductor-metal hybrid nanostructures are one of the best model catalysts for understanding photocatalytic hydrogen generation. To investigate the optimal structure of metal co-catalysts, metal-CdSe-metal nanodumbbells were synthesized with three distinct sets of metal tips, Pt-CdSe-Pt, Au-CdSe-Au, and Au-CdSe-Pt. Photoelectrochemical responses and transient absorption spectra showed that the competition between the charge recombination at the metal-CdSe interface and the water reduction on the metal surface is a detrimental factor for the apparent hydrogen evolution rate. For instance, a large recombination rate (k_{rec}) at the Pt-CdSe interface limits the quantum yield of hydrogen generation despite a superior water reduction rate (k_{WR}) on the Pt surface. To suppress the recombination process, Pt was selectively deposited onto the Au tips of Au-CdSe-Au nanodumbbells, in which the k_{rec} was diminished at the Au-CdSe interface, and the large k_{WR} was maintained on the Pt surface. As a result, the optimal structure of the Pt-coated Au-CdSe-Au nanodumbbells reached a quantum yield of 4.84%. These findings successfully demonstrate that the rational design of a metal co-catalyst and metal-semiconductor interface can additionally enhance the catalytic performance of the photochemical hydrogen generation reactions.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-430**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Production of Iron Oxides via Selective Extraction from a Mixed Chloride Solution

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An environmentally benign method for the selective separation of iron species from a mixed chloride solution containing Fe^{3+} , Mn^{2+} , Al^{3+} , Mg^{2+} , and Cr^{2+} ions by the pH-swing method was developed. The extraction process is carried out using aqueous NaOH solution. No organic toxic extractants were added. The method was evaluated for the selective precipitation of iron species from the mixed chloride solution. The precipitates were readily converted into iron oxide (Fe_2O_3) when they are annealed in air at 600 °C. Maximum extraction percentage of iron species is 96.27%, which is accomplished at pH = 10. Products were characterized by ICP-MS, X-ray powder diffraction, Transmission electron microscopy, UV-visible spectroscopy, X-ray photoelectron spectroscopy, and CIE 1931 color space. In addition, the possibility to extract other metal ions has been investigated but the extraction percentages of these elements are very low in the tested pH range.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-431**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Silica Coated Au-Ni-Au Nanorods for Drug Releasing System by External Magnetic Field

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¹*Department of Energy Science, Sungkyunkwan University, Korea*

Currently, a demand for controllable drug releasing platform is increasing. For precise drug releasing system, accurate modulation of releasing spot, the amount of drug and releasing rate with external stimuli are strongly required. Specifically magnetic nanostructure has been extensively researched since it is practicable in human body and reacts in real time. On the other hand, silica has also been widely explored as drug delivery vehicles due to their properties such as stability, uniformity and biocompatibility. However, combinatorial systems utilizing magnetic, plasmonic with silica coating are quite limited due to synthetic difficulty. Here, to overcome the limitation, we synthesized plasmonic-magnetic nanorods coated with silica shell by electrochemical deposition method with the help of anodized aluminum templates. Designed nanostructure enables to magnetically control drug releasing system, realized by an external magnetic field. Furthermore, the presence of plasmonic segment can enhance the light to heat conversion due to localized surface plasmon resonance. By controlling the silica thickness, nanorod length and rotating speeds of external magnetic field, we investigated the effect of magnetic field on releasing rate in drug releasing system. The result indicates that releasing rate is dependent upon rotating speeds of external magnetic field and silica thickness due to the increased amount of mass loading. Conclusively, Silica coated Nanorods composed of plasmonic-magnetic segments have distinct enhancement of drug loading capacity and releasing rate comparing with bare nanorods without coating silica. We expect this study will contribute to the understanding the control of nanomaterials and therapeutic nanosystems.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-432**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Trimetallic Au@PdPt Tip-Hollow Octahedron through Nanoscale Kirkendall Effect and Their Catalytic Properties

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The synthesis of multimetallic nanoparticles (NPs) is critical for designing highly active and durable catalyst and for investigating their possible applications. Herein, we report a facile synthesis of trimetallic Au@PdPt octahedral NPs with hollow cavities. These cavities are located in six vertex of octahedral shape, and we successfully made this tip-hollow nanostructure by diffusing inner Au at 100 °C. This high temperature is main condition of Kirkendall effect. In this synthesis process, nanoscale Kirkendall effect make cavities in the vertex of NPs called Kirkendall void. These cavities made large surface to volume ratio into the NPs. So, the prepared NPs showed excellent catalytic performance for electrooxidation (methanol, ethanol, CO) which can be attributed to their optimized binding strength toward adsorbate molecules.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-433**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of Tip-blobbed Au Nanoframe Structures and Their Photothermal performance

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Hollow Au nanostructures have gained considerable attention in biomedical applications such as photothermal therapy because of their localized surface plasmon resonance (LSPR) in the NIR region (600 nm~900 nm). Most of hollow Au nanostructures through galvanic replacement reaction (between silver nanocrystals and Au ions) have disadvantages which contain silver components with cytotoxicity and difficult to precise control of final morphology and the LSPR peak position. In this paper, we synthesized Tip-blobbed pure Au nanoframe (TBNF) structures and study their photothermal effect in vitro and stability in harsh chemical environment. In Au regrowth step, Au ions preferably deposited on tip sites of Pt frame because Au-Au lattice mismatch is lower than Au-Pt lattice mismatch. By using the Pt frame as a template, we could be precisely controlling rims thickness of TBNFs and have good structure rigidity. These TBNFs displayed an attractive photothermal conversion ability and great photothermal stability, and could efficiently kill Hela cancer cells through light-induced heating. These results suggest that this new class of Au hollow structures, Tip-blobbed Pure Au nanoframes, can potentially serve as an effective photothermal therapeutic agent for cancer treatment.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-434**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Octahedral Rhenium Sulfite Clusters as New Materials for Solar Cell

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In recent years, there has been increasing interest in photoluminescent octahedral clusters [$\{M_6Q_8\}L_6$] (where M is Mo, W or Re; Q – inner ligands) materials. In particular, hexanuclear rhenium(III) cluster complexes with wide variety of chemical and physical properties are the most potential candidate among the family of rhenium cluster compounds. Because of excellent photoluminescent properties, octahedral rhenium clusters are significant materials for various applications, such as solar cell, light emitting and biological application. In the present study, the new cluster $[Re_6Q_8(TBP)_5(SO_3)]$ (where Q is Se or S) was synthesized and characterized. The structures were confirmed by chemical analysis and energy-dispersive X-ray spectroscopy methods.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-435**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis and controlled release properties of Zn-Al layered double hydroxide hybrid composite

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Department of Chemistry, Changwon National University, Korea

A hybrid composite between Zn-Al layered double hydroxide (LDH) and herbicides glyphosate (GLY) or 2,4-dichlorophenoxyacetic acid (2,4D) were prepared for study slow/controlled release. Compared to the physically mixing, these hybrid composite displayed slow-release properties in decarbonated distilled water. The release rate of herbicides was found to be dependent on the carbonate and chloride anion concentrations in solution. The time at which 50% of the herbicides were released from the hybrid composite into solution, t_{50} , ranged from 6.5 to 18.6 h for LDH-GLY and from 10 to 21.5 h for LDH-2,4D. These results confirm that the application of LDH-GLY or LDH-2,4D hybrid composite to agricultural areas could reduce the maximum 2,4D or GLY contamination and result in the retardation of herbicides leaching through the soil. This study demonstrates the potential applicability of LDHs as supports for the slow release of acid herbicides

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-436**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Amphiphilic Alginate Functionalized Upconversion Nanoparticles for Highly Efficient pH-Responsive Drug Delivery

**Salah Mahmoud Tawfik Ahmed, SHARIPOV MIRKOMIL, Huy B.T., Zayakhuu
Gerelkhuu, YONG-ILL LEE***

Department of Chemistry, Changwon National University, Korea

Novel amphiphilic alginate polymers were synthesized to act as functionalizing agents for upconversion nanoparticles (UCNPs). The synthesized amphiphilic alginate functionalized UCNPs show high stability, excellent biocompatibility and enhanced luminescence intensity. Additionally, our results show that due to the large cavities of the materials and amphiphilic polymer shell, these amphiphilic alginate functionalized UCNPs were able to load the anticancer drug doxorubicin (DOX) with the excellent efficiency as well as release it in a highly controlled and selective pH-responsive manner via folate receptor-mediated endocytosis. Targeting using this amphiphilic alginate significantly improved the capability of DOX-loaded UCNPs to inhibit the growth of KB cancer cells than free DOX. These biocompatible amphiphilic alginate functionalized UCNPs hold substantial potential as effective anticancer drug-delivery carriers

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-437**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Design and Synthesis of TiO₂ nano particles involving acetyl acetone derivatives for Electron Transfer Layer of Solar Cell

Habin Sim, Hyerim Oh¹, Wonsuk Kim^{2,*}

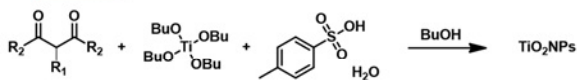
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A solar cell is an electrical device that converts the energy of light to electricity by the photovoltaic effect, which is a physical and chemical effects. Solar cells are regarded as one of the key technologies towards a sustainable energy supply. Therefore, numerous solar cells have been reported about efficiency. Herein, we report new TiO₂ nano particles containing acetyl acetone derivatives for electron transfer layer of solar cell. They showed the differences in the stability during light soaking under 1 sun. Among the synthesized TiO₂ nanoparticles, the most stable device TiO₂ nanoparticle showed 6.68% efficiency after 400 h light soaking, representing the only 26% of the efficiency decrease compared to as-fabricated device.

TiO₂ NanoParticles Synthesis condition



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Code: **MAT.P-438**

Area: Material Chemistry

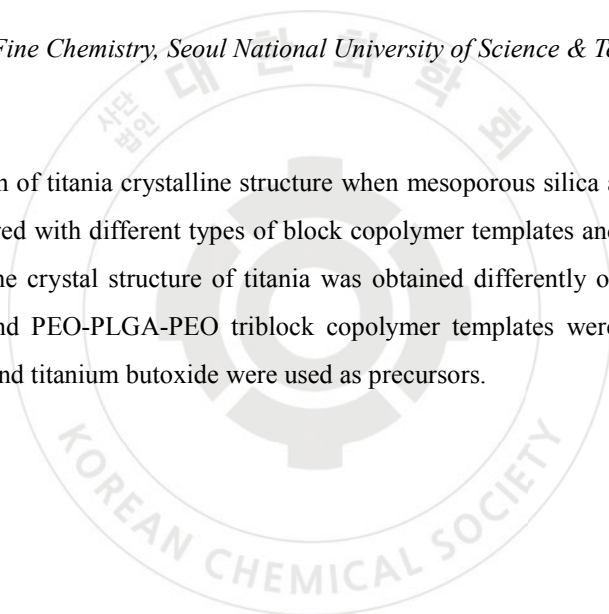
Type: Poster Presentation, Time: THU 11:00~12:30

Variation of Titania Crystalline Structure During Sol-Gel Synthesis of Ordered Mesoporous Silica and Organosilica

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We present the variation of titania crystalline structure when mesoporous silica and periodic mesoporous organosilicas are prepared with different types of block copolymer templates and organosilica precursors in acidic conditions. The crystal structure of titania was obtained differently on chemicals used in this study. Typical P123 and PEO-PLGA-PEO triblock copolymer templates were used as templates and TEOS, BTEE, BTEB, and titanium butoxide were used as precursors.



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Code: **MAT.P-439**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Enhanced Photoelectrochemical Water Oxidation Efficiency of ZnO Photoanodes by Forming Heterojunctions

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Department of Applied Chemistry, Kyung Hee University, Korea

In the fields of photo-electrochemical (PEC) water splitting, heterojunctions in semiconductors often introduced to improve the efficiency and stability of PEC electrodes. For examples, buried junction formation using thin layer ZnS on Cu₂O can improve photoreduction currents compared to single Cu₂O. In this poster, we present formation of ZnO/ZnWO₄ heterojunction formation that show stability and efficiency enhancements. One-dimensional ZnO nanorods (NR) have been heavily studied as photoanodes due to its unique optical properties and higher electron mobility compared to other oxides. However, water splitting efficiency of ZnO is far lower than other oxides due to the chemical instability and the high recombination. In this poster, a core-shell photoanodes with ZnO NRs as a core and ZnWO₄ as a shell (denoted as ZnO@ZnWO₄) are synthesized by depositing WO₃ on hydrothermally grown ZnO NRs through thermal CVD process. For ZnO@ZnWO₄, stability and PEC performances are enhanced compared to pristine ZnO NRs, and we conclude that the enhancement are originated due to the improvement in charge transfer efficiency based on systematic optical and electrochemical analyses.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-440**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis of novel mononuclear Ru(II) complexes and dinuclear Ru(II) complexes containing bridging ligand for DSSCs

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¹*ST Pharm, Korea*

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Technologies using green energy have been developed through a lot of methods. Among them, the dye-sensitized solar cells (DSSCs) have been considered as a superior technology to convert solar energy into electrical energy. Expecting higher power conversion efficiency, a various heteroleptic Ru(II) complexes were developed to increase the photocurrent by using the various ligands. Kumar et al. also showed that dinuclear complex is more efficient than that of mononuclear complex by 1.7 times. Along with continuous development for more efficient DSSCs materials, we have newly prepared new heteroleptic Ru(II) complexes. Mononuclear Ru(II) complexes with α -diimine anchoring ligand (4,4'-dicarboxy-2,2'-bipyridine (bpy) or its conjugated derivative) and an ancillary ligand (4,4'-bis(E-styryl)-2,2'-bipyridine (bsbpy)) were synthesized. Likewise, dinuclear Ru(II) complexes with α -diimine anchoring ligand and bridging ligand (5-(2-[2,2'-bipyridin]-5-ylethynyl)-2,2'-bipyridine) were synthesized to estimate the efficiency for DSSCs. Physical and photovoltaic properties were also examined. Compared with standard cell based on N719, DSSCs based on our developed complexes showed reasonable efficiencies.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-441**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Influence of process parameters for electroless Ni-P plating on carbon fiber heating elements

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¹*Extreme Materials Research Division, KCTECH, Korea*

Nowadays, the heating elements of car seat mostly used copper wire. However, the copper wire had many problems such as electromagnetic wave emission and disconnection as oxidation and physical damage. Carbon fibers (CFs) compared to copper wire had many advantages such as far infrared radiation, corrosion resistance, and high mechanical properties. But, CFs had a low electrical conductivity compared to the copper wire. In this study, we were electroless plating due to the low electric conductivity of CFs. And we were investigated the heating performance of CFs and nickel plated CFs (NiCFs) with different pH, length, heat treatment time. The surface morphology and specific resistance of CFs and NiCFs measured by scanning electron microscope (SEM) and 4-probe method, respectively. The resistance and current measured by multimeter and power supply, respectively. The specific heat and residue distribution of CFs and NiCFs investigated by differential scanning calorimetry (DSC) and thermogravimetric analyzer (TGA), respectively. And the surface temperature of CFs and NiCFs measured by thermo-graphic camera with different process parameters.

Conference Date: October 18~20, 2017

Venue: Kimdajejung Convention Center, Gwangju

Code: **MAT.P-442**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Paper-based DMF chip with integrated heater and temperature sensor by all-in-one inkjet materials printing

YUNPYO KIM, Haena Cheong, Oh-Sun Kwon^{*}, Kwanwoo Shin^{*}

Department of Chemistry, Sogang University, Korea

Thermal heating and monitoring temperature of digital microfluidic (DMF) lab-on-a-chip on paper substrates has previously been investigated. In order to actuate a droplet on DMF paper chip, a rail pattern of electrodes (Fig. 1) was printed using an inkjet printer, Dimatix, with silver nanoparticle (AgNP) ink. Furthermore, a pair of heaters enclosing a temperature sensor was printed on the electrodes positions, forming the heating zone, as shown in Fig. 1, so that those three electrodes have simultaneous roles of: 1) actuated electrodes for DMF, 2) heater electrodes, and 3) temperature sensing electrodes. The temperature sensor was fabricated by printing the thermoelectric (TE) material, p-type PEDOT:PSS with AgNP electrode, forming the interfacial junction (inset in Fig. 1). As a result of depositing these two materials with Dimatix, the once printed AgNP layer was $1 \cdot \text{m}$ and the fifth printed PEDOT:PSS layer was $2 \cdot \text{m}$ (Fig. 2). This integrated configuration enables the thermal cycling process, heating and cooling, in addition to the DMF five normal mechanical operations of dispensing, merging, mixing, splitting and transporting. The sensor showed a linear response with a Seebeck coefficient of $23.051 \cdot \mu\text{V}/\text{K}$; demonstrating good usage as a temperature sensor for a DMF drop with on-chip monitoring. Furthermore, biochemical experiments will be conducted using the integrated heater-sensor DMF chip.

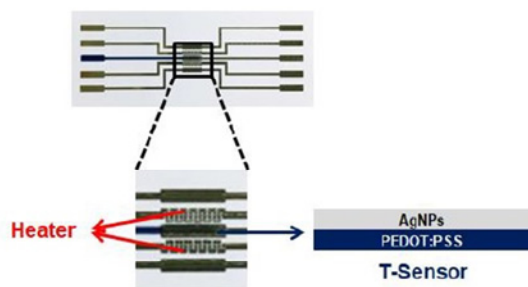


Fig. 1 Fabrication of a DMF paper chip with integrated temperature sensor and heater by material printing method only.

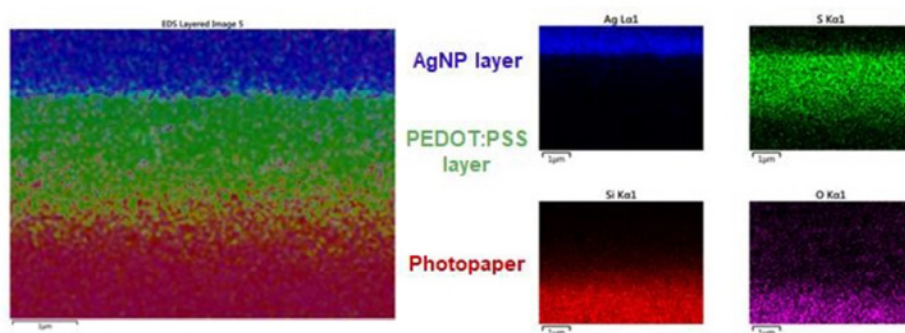


Fig. 2 Thickness of two materials measured with a SEM equipment, AgNP layer and PEDOT:PSS layer printed with Dimatix.



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Code: **MAT.P-443**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Evaluation of [18F]-Ganestepib as PET Imaging Agent Targeting HSP90 for Triple Negative Breast Cancer

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HSP90 is a molecular chaperone which is involved in the activation or stabilization of various cancer-inducing factors, called client proteins, for growth and proliferation of cancer cells, and has been reported to be overexpressed in various cancer cells. Oncogenic mutation and expression of client proteins requires the increased activity of HSP90 and results in overexpression of HSP90, which means the increased expression level of HSP90 is a common phenotype in human cancer. Client proteins of HSP90 have been widely discovered and includes various transcriptional factors such as HIF-1 α , receptor kinases containing ErbB2, intracellular kinases like Met tyrosine kinases, MEK 1/2 and CDKs as well as steroid hormone receptors, telomerase, metalloproteins, Src, Akt and Raf-1. All of these client proteins exist in various signaling pathways for the survival, proliferation, invasion, metastasis, and angiogenesis of cells and are known to contribute to the malignancy of cells. A lot of HSP90 inhibitors such as geldanamycin (GA), 17-AAG, 5-PU and ganetespib have been developed for therapeutic purpose in clinical trials. In particular, ganetespib has discovered that it has no side effects shown in most HSP90 inhibitors containing GA, 17-AAG and other HSP90 inhibitor, and is currently conducting a Phase 3 clinical trial. Ganetespib which has been discovered by Synta Inc, showed a tumor uptake to be over 20 times higher than normal tissues in clinical trial as well as xenograft mouse model, which implies ganetespib is a strong candidate as a ligand for PET imaging agent. On the basis of these reports, we synthesized ganetespib derivative as a HSP90 ligand and introduce 18F radioactive isotope by click chemistry for PET imaging of cancer. Cell uptakes of [18F]-ganetespib in MDA-MB-231, MCF-7, SK-BR3 and A549 cell lines were performed, and MDA-MB-231, triple negative breast cancer cell lines, showed a good cell uptake of [18F]-ganetespib. We are currently under in vivo evaluation of [18F]-ganetespib in skin and orthotopic xenograft mouse model.

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Code: **MAT.P-444**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Graphitic carbon nitride as efficient metal-free photocatalysts for hydrogen evolution reaction and their dependences on grain size, porosity, chemical structure, and photophysical properties

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Three-dimensional (3D) graphitic carbon nitride (g-C₃N₄) based materials show excellent performance in hydrogen evolution reaction (HER). C₃N₄-based materials have generated research interest as possible efficient, low cost, and environment-friendly photocatalysts for HER. In this work, we characterized dependences of the photocatalytic natures of g-C₃N₄ materials on grain size, porosity, and size distribution of Pt nanoparticles as co-catalysts. We produce a series of g-C₃N₄ materials on synthetic approaches (precursor type, temperature, time, and the gaseous environment). HER catalytic activity is affected by the surface area, the presence of amine groups, and the distribution of small sized Pt nanoparticles. Also, photocatalytic activities depend on the band gaps and lifetimes of photogenerated charge carriers. We have examined the relationships of the factors mentioned above, urea driven g-C₃N₄ produced in a N₂ atmosphere is found to exhibit the best photocatalytic activity (up to 130 mol h⁻¹ g⁻¹).

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Neurite Outgrowth of Hippocampal Neurons on Patterned Silica Bead Arrays

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Neurite outgrowth and path-finding behaviors of neurons is an important preceding step for the development of nerve systems. These are governed by two protrusive, actin-based molecular structures, filopodia and lamellipodia, the diameter of which is generally in the range of 100-300 nm. The dynamic stability of filopodia and lamellipodia allows neuronal cells to recognize the surrounding environments at the nanometer scale and to subsequently modify their cytoskeletal structures in response to stimuli/cues. Given that the in vivo environments of neurons consist of numerous hierarchical micro/nanotopographies, there have been many efforts to investigate the relationship between neuronal behaviors and surface topography. In this study, we investigated the effects of the orientation of nanotopographies on the neuronal development and neurite outgrowth using patterned silica bead arrays. The silica beads were synthesized by stöber method and assembled by rubbing method. In particular, we can obtain the both the hexagonally and tetragonally close-packed silica bead arrays using template assisted rubbing method. The initial hippocampal neurons become to accelerate their neurite outgrowth on close-packed silica bead arrays due to tension-induced developmental acceleration. The neuronal networks were formed randomly on the hexagonally close-packed silica bead arrays, whereas they were aligned bidirectionally along to the orientation of tetragonally close-packed silica bead arrays.

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Code: **MAT.P-446**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Layer Controlled MOCVD Growth of WS₂ films by Sulfurization of W film

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Transitional metal dichalcogenides (TMDC) are interested due to their electronic, optical properties like conductivity and band gap. Synthesis of TMDC like MoS₂ and WS₂ through the CVD method has researched variously. However, there is a limit to the difficulty of controlling the thickness. To complement the limitations, many advanced CVD methods for forming TMDC by forming a transitional metal film and then reacting with chalcogenide source by CVD have been studied. Especially, among the methods of depositing the metal like sputter and lithography, the atomic layer deposition (ALD) is most excellent because it can be formed thinly up to the monolayer. And beyond the CVD method, the metal organic chemical vapor deposition (MOCVD) method can quantitatively adjust the amount of source through mass flow controller (MFC). Here, we present the preparation of the WS₂ films via MOCVD method using tungsten film deposited by ALD and diethyl sulfide (S(C₂H₅)₂) on silicon oxide wafer and characterized by atomic force microscopy (AFM). We observed two main Raman modes peaks of WS₂, using micro-Raman spectroscopy and show band gaps by photoluminescence measurement. And we investigated their conductivity through the 4-point probe measurement. Reference [1] Song, J-G.; Ryu, G. H.; Lee, S. J.; Sim, S.; Lee, C. W.; Choi, T.; Jung, H.; Kim, Y.; Lee, Z.; Myoung, J-M.; Dussarrat, C.; Lansalot-Matras, C.; Park, J.; Choi, H.; Kim, H. Nature. Comms. 2015, 6, 7817. [2] Song, J-G.; Park, J.; Lee, W.; Choi, T.; Jung, H.; Lee, C. W.; Hwang, S-H.; Myoung, J. M.; Jung, J-H.; Kim, S-H.; Lansalot-Matras, C.; and Kim, H. Sci. Report. 2013, 7, 12, 11333-11340.

Conference Date: October 18~20, 2017

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Novel Activated Carbon Surface Treatment for Improving CO₂ Adsorption Performance

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Conventionally, activated carbon is surface-treated with metal-based materials to achieve various gas adsorption performance as well as CO₂. However, in this study, the adsorption performance of CO₂ was maximized not only by the metal treatment but also by the amine functional treatment which can selectively adsorb CO₂. Barium and potassium were treated as a metal functional site and TEPA as an amine functional group. The treated activated carbon was analyzed by SEM-EDS, BET and XPS, and CO₂ adsorption performance was analyzed by GC with gas flow system. In the case of CO₂ adsorption performance, it was confirmed that the CO₂ adsorption performance was significantly increased when the amine was treated in the same way as the activated carbon which was treated only with the metal. This was because the functional group capable of adsorbing CO₂ was greatly increased not only in the metal but also in the amine group. It is considered.

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Code: **MAT.P-448**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Efficient Photocatalytic Activity of Cu and Ag Co-doped TiO₂ Hollow Sphere Composites for Methylene Blue under Visible Light Irradiation

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Department of Chemistry, Keimyung University, Korea

In this study, Cu and Ag co-doped TiO₂ hollow sphere (CATHS) composites were synthesized by using a range of 0 to 1.0 mol% via sol-gel method. CATHS composites were confirmed by X-ray diffraction (XRD), transmission electron microscopy (TEM), ultraviolet-visible diffuse reflectance spectroscopy (UV-DRS) and X-ray photoelectron spectroscopy (XPS). UV-DRS showed that the resulting co-doped TiO₂ composites broadened the absorption threshold to the visible light region, compared to pure TiO₂. The stability of anatase phase was increased with co-doping of silver and copper to TiO₂ lattice. The photocatalytic activity of all samples were evaluated in the photocatalytic degradation of methylene blue (MB) under visible-light irradiation. The results showed that co-doped TiO₂ composites can effectively degrade MB, and that it is an excellent photocatalytic enhancement than pure TiO₂.

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Code: **MAT.P-449**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Curvature-Dependent Surface Potentials of Zincone Films Grown by Molecular Layer Deposition

Ui-Jin Choi, Hyemi Lee, JIN SEOK LEE*

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 process is based on self-saturating 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), we confirmed the different growth behavior of zincone films grown on curvature substrates with different ratio. And, we investigated their curvature-dependent surface potentials by performing ex situ analysis using scanning kelvin probe microscopy (SKPM). Furthermore, their molecular geometries and energies on substrates with various curvatures were predicted by performing density functional theory (DFT) calculations.

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Code: **MAT.P-450**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Photo-switching Behavior of Azobenzene-Containing Polyamide Films Grown by Molecular Layer Deposition

uijin choi, Hyemi Lee, JIN SEOK LEE*

Department of Chemistry, Sookmyung Women's University, Korea

Photo-sensitive polymer film has been attracted in the field of material science including biological system and optical devices 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 in the research related photo-sensitive polymer film including surface science, artificial muscle, biological and optical application, because light used as external triggers for inducing surface transformation is manageable to control without modification of nano-structures and environment concerns. In this study, we fabricated photo-switchable polyamide films by molecular layer deposition based on sequential and self-limiting surface reaction between azobenzene-4, 4'-dicarbonyl dichloride (Azo) and organic diamines, such as phenylenediamine (PDA) and hexamethylenediamine (HDA). And, we investigated the photo-induced reversible transformation of azobenzene-containing polyamide thin film. In situ Fourier Transform Infrared (FTIR) measurement was used to monitor the growth of corresponding polyamide films, and the photo-switching behavior of surface topography was characterized by Atomic Force Microscopy (AFM). Also, to predict the orientation of functional groups in azobenzene-containing polyamide film, we investigated the angle dependence of each IR peaks using a plan-polarized grazing angle FTIR spectroscopy. Reference [1] J. S. Lee; Y. -J. Lee; E. L. Tae; Y. S. Park; K. B. Yoon, *Science*, 2003, 301, 818–821. [2] N. M. Adamczyk. A. A. Dameron. and S. M. George. *Langmuir* 2008, 4, 2081-2089. [3] Y.-S. Park, S.-E. Choi, H. Kim, J. S. Lee, *ACS Applied Materials & Interfaces*, 2016, 8 (18), 11788–11795. [4] D. Liu and D. J. Broer. *Nature Comm.* 2015, 6, 8334.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-451**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly Emissive Octahedral Molybdenum Metal Cluster-Polymer Hybrid and Application on Large Window

DIEU NGUYEN, SUNGJIN KIM^{1,*}

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

Recently, luminescent solar concentrator (LSC) is promising candidate for BIPV application due to many its advantages, especially it is a very flexible in its design with a variety of possible shapes and colours and it has very high transparency. Additionally, it has low cost and very stable in ambient air. LSC as a complement to conventional photovoltaic cell (PVC), involves many luminophores absorb incident light and isotopically emit absorbed incident lights at longer wavelengths. These emitted lights be captured by a small attached-PVCs (Si-cells) at the edge waveguide, this PV cell will capture and convert emitted lights into electricity we report a very simple process was realized in the air ambient with very transparency near 90% and attained efficiency of up to 1.2-1.65% depending on various concentration with the highest efficiency of 1.65%.

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Code: **MAT.P-452**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Pt Adsorbed Metal-Organic Framework and Its Conversion to Pt Doped Co@Carbon Composites

Euisoo Kim, Minyoung Yoon*

Department of Nanochemistry, Gachon University Global Campus, Korea

Metal nanoparticle embedded porous carbon composite materials can be used in a variety of application area, including catalyst supports, sensors, and adsorbents due to their high stability and unique porosity. Porous carbon composite materials can be prepared using various synthetic methods, recent efforts provide a facile way to prepare the composites from metal-organic frameworks (MOFs) by pyrolysis. We can usually get metal or metal oxide embedded porous carbon composites by MOF pyrolysis, but it is usually difficult to control the structure of the phase of metal or metal oxide during synthetic process. Among many kinds of MOFs, recently cobalt based MOFs draw attention because of unique catalytic and magnetic properties of the cobalt. Herein, we report preparation of a Pt metal nanoparticle embedded cobalt based MOF and their conversion into cobalt nanoparticle embedded porous carbon composites (Pt doped Co@C). Interestingly, the phase of cobalt metal nanoparticles (FCC and HCP) can be controlled by the change of a synthetic condition. The prepared Pt doped Co@C was characterized by XRD, gas sorption analysis, TGA, and XPS. In addition, catalytic activity of the composite for CO₂ conversion is now in progress. Further details of this work will be presented.

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Code: **MAT.P-453**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Up/Down-conversion luminescence properties of GdNbO₄:Yb³⁺, Er³⁺ phosphor materials by various Er³⁺ ions concentrations

Jong Won Chung, Zayakhuu Gerelkhuu, Da Som Jung, YONG-ILL LEE*

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Recently, up-conversion phosphors(UCPs) are concentrated in the research of luminescent materials, because of their potential applications, such as flat panel display(FPD), photodynamic therapy and high resolution color display. Trivalent erbium ion is one of the most important activators for red and green emission phosphors. UC luminescence of rare-earth doped phosphor has been extensively investigated. Effective way of generating light is the UC that converts from near infrared(NIR) photons to visible photons through multi photon processes. Coupled with an infrared(IR) rays excitation light source which low auto-background, high resistance to photo-bleaching and high penetration depth tissue, UCPs emitting the visible spectrum have offered the substantially potential benefits in nano-materials, ultrafine powders, volumetric displays, temperature sensors, photo dynamic therapy and biological imaging agents, compared with other solid-state lighting such as down-converted phosphors. In addition, there is an increasing need in dense, fast and bright scintillators for high energy physics, medical diagnostics and security screening devices. Recently, some new efforts have been made in study of scintillation characteristics of compounds with the common formula ABO₄, where (A: rare earth ion, B: the V group elements-V, Nb or Ta). In this report, the GdNbO₄:Yb³⁺, Er³⁺ phosphors were synthesized by facile solid state reaction to investigate its luminescent properties. The x-ray diffraction (XRD), field scanning electron microscopy (FE-SEM), photo luminescence (PL, down conversion) and up-conversion (UP) of GdNbO₄:Yb³⁺, Er³⁺ phosphors have been measured and the relationship between the properties discussed.

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Code: **MAT.P-454**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Study on Li⁺ conductivity and phase stability of doped Li₂(OH)_{0.9}X_{0.1}Cl (X=F, Br) electrolyte for lithium metal anode in lithium metal batteries

YongSeok Lee, Kwang Sun Ryu^{*}

Department of Chemistry, University of Ulsan, Korea

Recently, Li₃OX (X=Cl, Br) called antiperovskite electrolyte have been studied because the materials have low melting point and high electrochemical stability. The materials have shown but also low interface resistance causing good ionic conductivity and the good anodic stability which can be applied to lithium metal. However, the materials have synthesis problem. On the other hand, Li₂OHX have some advantages such as easy one step synthesis, low cost, and high stability except for lower ionic conductivity than Li₃OX. For developing low ionic conductivity of Li₂OHX, John B. Goodenough et al. had studied Li₂(OH)_{1-x}F_xCl, which was F doped in OH site. Because fluorine has smaller ionic size than Cl, substitution of F in OH site not only reduces the concentration of H⁺ hindering Li⁺ diffusion but also induces the larger size of the cavity composed with Cl-O-Cl hole. As the results, the Li⁺ conductivity of Li₂OH_{1-x}F_xCl was improved. Based on above studies, we have investigated X doped Li₂(OH)_{0.9}X_{0.1}Cl (X=F, Br) to study the size effect of the substitution with F and Br each having smaller and larger size than Cl. Also, we have compared with the electrochemical stability by the strength of ionic bonds according to halogen ions. The materials were synthesized by using a solid-state method and compared with the crystal structures and ionic bonds by XRD and FT-IR. The morphologies and contents of the elements in the materials were analyzed by SEM and EDS. As the electrochemical analysis, electrochemical impedance spectroscopy with various temperatures was conducted to evaluate Li⁺ conductivity of the materials. For analysis of electrochemical versus Li metal, cyclic voltammetry and DC-cycling tests were conducted with a current density of 1.0mAcm⁻².

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Area: Material Chemistry

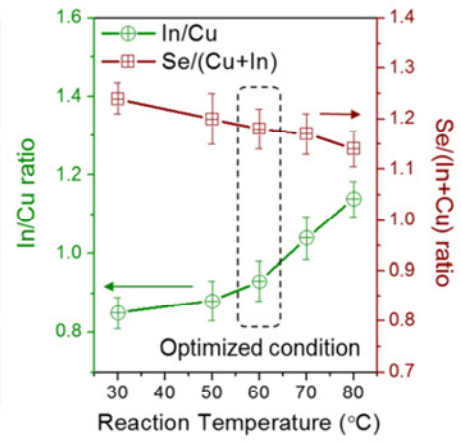
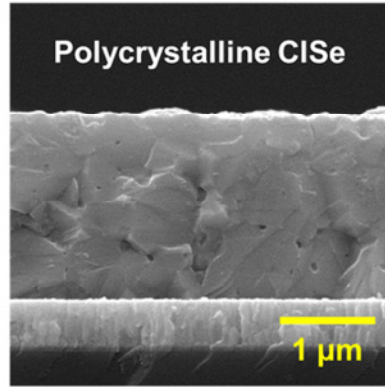
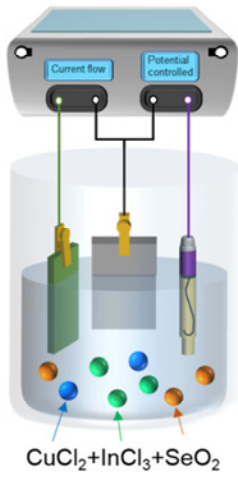
Type: Poster Presentation, Time: THU 11:00~12:30

Effect of Complexing Agent and Reaction Temperature on the One-Step Electrochemical Deposition of CuInSe₂ Thin Films

Ji-Hyun Cha, Seonho Jung, HyunJong Lee, Duk-Young Jung*

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Highly dense and large grain size CuInSe₂ (CISE) polycrystalline thin films were synthesized by one-step electrochemical deposition under ambient atmosphere using oxalic acid and glycine as complexing agents. Three compounds, CuCl₂, InCl₃, and SeO₂, as precursors were used with glycine or oxalic acid as complexing agents. The major issues of CISE electrochemical deposition are the control of the chemical compositions and surface morphology of CISE precursor layers for high-quality absorber layers. To achieve the ideal stoichiometry and uniform deposition of CISE thin films, the reaction temperature and acidity of precursor solution were investigated. As the reaction temperature increased, Cu deficiency in the CISE thin film was observed. The density and surface morphology of CISE films prepared by one-step electrodeposition were affected strongly by the acidity of deposition solution, and addition of HCl in the solution improved the density and surface roughness of as-deposited CISE films. Denser and larger grain size CISE polycrystalline films prepared in oxalic acid solution. Two-step heat treatments for the prepared CISE samples were applied for fabrication of the CISE photovoltaic devices without additional Se source.



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Code: **MAT.P-456**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Cytochrome C conjugated DNA-gold nanoparticles for pH-responsive aggregation and its applications for photothermal therapy of cancer cells

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Stimuli-responsive gold nanoparticles(AuNPs) was extensively studied for a wide range of applications in different research fields. Here, we report a pH-responsive DNA conjugated AuNPs. We synthesized cytochrome c conjugated DNA-AuNP by binding double-stranded DNA and Cytochrome c to AuNPs. Cytochrome c is a zwitterionic polymer with an isoelectric point of about 6.8 and contains many cysteines that can be covalently conjugated to AuNPs. When the pH of a solution containing cytochrome c conjugated DNA-AuNPs was changed from 7.4 to 6.0, the color and optical properties of the solution change because the cytochrome c conjugated DNA-AuNPs aggregate. By controlling the ratio of cytochrome c conjugated to AuNPs, the pH being aggregated can be controlled. When the pH of the solution returns to 7.4, the color and optical properties of the solution are reversibly returned. Next, we exposed cytochrome c conjugated DNA-AuNPs to a 660 nm laser for photothermal therapy. DNA-AuNPs conjugated to cytochrome c exposed to laser generated heat. These reversibly aggregated DNA conjugated AuNPs may be applied for photothermal therapies.

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Code: **MAT.P-457**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Nanoscale DNA hydrogel as a template for optical properties of AuNP

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The DNA and gold nanoparticles (AuNPs) have been used for various researches and applications. Specially, as AuNPs are associated with DNA, AuNPs can have desired properties and be used to the novel applications. It is well known that DNA can be used as a building block that can make sophisticated and diverse structures by using the complementary base pairing of DNA. DNA hydrogel (Dgel) is a structure utilizing this DNA characteristic. In this study, we have varied the concentration and the base number of strands of X-DNA for the tunable properties of Dgel. As a result, the low molar concentration or more base numbers of X-DNA, the larger size Dgel was produced. Unique optical properties of AuNPs were attributed to localized surface plasmon resonance. Dgel was used to a template for assembling AuNPs as electrostatic interaction between negative charge of Dgel and positive ligand capped AuNPs (ligand-exchanged using quaternary ammonium molecules). Dgel-AuNPs assemblies exhibit more diverse optical properties through variously synthesized Dgel. Because the interparticle distance of AuNPs on Dgel varies depending on the size or space of Dgel, the larger size Dgel resulted to wider spacing among the AuNPs. The Dgel-AuNP assemblies were characterized by absorbance, hydrodynamic size, scanning electron microscopy measurement. These results suggest that the Dgel-AuNPs complex can be shifted for desired properties by controlling Dgel as the template.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Improved Electrochemical Performance of Carbon-Coated ZnO Microspheres as an Anode Material for Lithium-Ion Batteries

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Department of Chemistry, Dong-A University, Korea

Metal oxides have been widely studied as alternative anode material for lithium ion batteries (LIBs) because of their theoretical capacity higher than that of the commercialized graphite anode (about 372 mAh g⁻¹). Among them, zinc oxide (ZnO) has advantages of natural abundance, low cost, non-toxic, and a high theoretical capacity (978 mAh g⁻¹) through the alloy and conversion reactions of ZnO with lithium ions. Despite these advantages, ZnO has low electrical conductivity, slow diffusion of lithium-ion, and large volume changes during charge/discharge processes, which lead to severe capacity fading and poor reaction kinetics. In this study, carbon coated ZnO microspheres were synthesized through hydrothermal reaction using ethanol as solvent and maleopimaric acid (MPA) or abietic acid (A) as carbon source, respectively. To compare the ligand effects of carboxyl groups with Zn ion, the number of carboxyl groups was controlled by using natural rosin derivatives MPA and A. Compared to A-ZnO and bare ZnO, MPA-ZnO show a higher discharge capacity of about 763 mAhg⁻¹ after 100 cycles at a rate of 0.1 C in the voltage range of 0.01-3.0 V.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ionic Conductivity of Polymer Electrolyte Dependent on the Morphology of Fillers and Development of Flexible Electrochemical Gas Sensor

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Since polymer electrolytes are flexible, they can be easily applied to construct flexible electrochemical gas sensors. However, generally the ionic conductivity of polymer electrolytes is not enough to apply them to practical devices. So far, numerous efforts have been tried to increase the ionic conductivity of polymer electrolytes by adding various plasticizers and fillers. For example, S. N. S. Begum et al. added gold nanoparticles into chitosan-based polymer electrolytes, and observed enhanced ion conductivity. As another example, W. Liu et al. used ceramic nanowires or nanospheres as fillers to make polyacrylonitrile-based polymer electrolytes, respectively. And they found that the ionic conductivity of polymer electrolytes containing nanowires is higher than that containing nanospheres. Herein, we synthesized metal nanoparticles of various shapes (sphere, wire et al.) and used them as additives of polymer electrolytes for development of flexible electrochemical gas sensors.

$\text{Polymer} + \text{Ag}^+ \left[\begin{array}{c} \text{O} \\ \parallel \\ \text{O} \text{---} \text{N} \text{---} \text{O} \\ | \\ \text{O} \end{array} \right]^-$

$\text{Polymer} + \text{Ag}^+ \left[\begin{array}{c} \text{O} \\ \parallel \\ \text{O} \text{---} \text{N} \text{---} \text{O} \\ | \\ \text{O} \end{array} \right]^- + \text{O}=\text{Cl}-\text{O}^- \text{Li}^+$

작동전극, 키트산 고체 전해질, 기판, 기준전극, 카운터전극, 외부 단자, 센서 측정



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-460**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Small Molecule based Hole Transport Layer in Colloidal Quantum Dot Solar Cells

Havid Aqoma, Muhibullah Al Mubarak, Wisnu Tantyo Hadmojo, Sung-Yeon Jang*

Chemistry, Kookmin University, Korea

Colloidal-quantum-dot (CQD) solar cells have a potential to be low-cost solar energy harvesting devices due to low-temperature solution processability and bandgap tunability. Much effort to improve quantum dot surface passivation, which resulted in less trap density, has enhanced the device performance. However, the hole-transport-layer (HTL) in CQD photovoltaic devices still have much room to further develop and improve the charge collection efficiency. Herein, we synthesis novel organic benzodithiophene-based small molecule (BDT4) as the HTL for CQD solar cells. We compared the performance of BDT4 with P3HT, which has been widely used as HTL for photovoltaic devices. The deeper HOMO level of BDT4 than P3HT promotes better hole-injection from CQD active layer to HTL, while improves built-in voltage of devices. This result reveals that the use of small molecule as HTL is a promising strategy to further improve charge collection efficiency in CQD photovoltaic devices.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-461**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

High Efficiency and Fullerene-Free Organic Solar Cells based on Wide Bandgap Polymer Donor and Narrow Bandgap Acceptor

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Nonfullerene organic solar cells (OSCs) has seen rapid development in the past several years and has reached > 10 % efficiency. However, there have been only several study that shows high performance fullerene-free OSC with low energy loss. We developed OSC based on a wide bandgap polymer donor and a narrow bandgap, small molecule acceptor, ITIC. The complementary absorption, well matched morphology, and the favorable optical, electronic, and energetic properties of the polymer donor with respect to ITIC achieved panchromatic photon-to-current conversion with PCE of 10 %.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-462**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Zinc oxide-copper(I) oxide colloidal nanoparticles as high performance photocatalyst for carbon dioxide conversion into methane

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Contemporary human is facing in many environmental problems such as exhaustion of fossil energy resources and global warming from greenhouse effect. To cope with environmental problems, efficient generation of alternative energy resources and reduction of greenhouse gas mainly CO₂ is necessary. In the environmental point of view, photocatalytic CO₂ conversion reaction is ideal and ultimate reactions. There are many another factor determine catalytic properties such as structures, morphology and interface of each components. However, there are few papers are reported using well-defined hybrid nanostructures for photocatalytic CO₂ reduction. In this study, we synthesized ZnO-Cu₂O colloidal nanoparticles and applied the nanoparticles to the photocatalytic CO₂ reduction. This catalyst exhibited high activity (1080 μmol gcat⁻¹ h⁻¹) and selectivity in methane production (>99%). The proper band alignment of ZnO and Cu₂O, and their well-defined structures and junctions lead to high catalytic performance.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-463**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Molybdenum Oxysulfide Electrocatalyst Prepared by Chemical Bath Deposition for Hydrogen Evolution Reaction

Seokhee Shin, ZHENYU JIN, Sunyoung Lee, Yo-Sep Min*

Department of Chemical Engineering, Konkuk University, Korea

Recently, MoS₂ has attracted great attention as an electrochemical catalyst for hydrogen evolution reaction (HER). MoS₂ electrochemical catalysts are usually doped with transition metals or chalcogen atoms to enhance catalytic activity. Here we report molybdenum oxysulfide catalysts prepared in liquid phase via chemical bath deposition for HER. The molybdenum oxysulfide catalysts are deposited at 90 °C on carbon fiber papers (CFP) in an aqueous solution of ammonium molybdate and thioacetamide as molybdenum and sulfur precursors, respectively. Sodium dithionite is added to the solution as a reducing agent for molybdate ions. Oxygen ratio of molybdenum oxysulfide is controlled by adjusting the concentration of reducing agent. The optimized catalyst exhibits an excellent cathodic current density of 10 mA/cm² at 166 mV vs. RHE. The Tafel slope and the exchange current density are 45.79 mV/dec and 2.37 μA/cm², respectively.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-464**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Investigation of Band Structure on Amorphous Zinc Tin Oxide Thin Films grown by Atomic Layer Deposition

Sunyoung Lee, ZHENYU JIN, Seokhee Shin, Yo-Sep Min*

Department of Chemical Engineering, Konkuk University, Korea

Thin film photovoltaic cells has required a buffer layer in a window layer stack to prevent unfavourable conduction band line-up which promotes interface recombination. Zinc tin oxide (ZTO) has recently attracted great attention as an alternative buffer layer, since this material exhibits some advantages over the existing CdS. However, their work function which is a essential parameter for band alignment at equilibrium has not been characterized in detail. Here, we investigated compositional, structural and optical characteristics of ZTO thin films to construct the band diagram for films with different Sn contents. ZTO films were grown at 150 °C by atomic layer deposition (ALD) using tetrakis(dimethylamido)tin(IV), diethylzinc, and water. The ZTO films were amorphous and exhibited wider optical bandgaps than that of CdS. Chemical structure and work function analyses were performed by X-ray photoelectron spectroscopy and Kelvin probe force microscopy, respectively. It indicated that the incorporation of Sn into ZnO strongly influenced the content of oxygen vacancies and work function which is related to carrier concentration. In addition, in order to confirm the validity of the constructed band diagrams, we investigated the diode characteristics of heterojunctions for n-ZnO/p-Si, n-SnO₂/p-Si and n-ZTO/p-Si. The band diagram of the ALD-ZTO films will be useful to understand the band alignment of a photovoltaic cell with a buffer layer of ZTO film such as CIGS solar cells.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-465**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Co-catalytic Effects of CoS₂ on the Activity of the MoS₂ Catalyst for Electrochemical Hydrogen Evolution

ZHENYU JIN, Seokhee Shin, Sunyoung Lee, Yo-Sep Min^{*}

Department of Chemical Engineering, Konkuk University, Korea

MoS₂ is a promising material to replace the Pt catalyst in the electrochemical hydrogen evolution reaction (HER). It is well known that the activity of the MoS₂ catalyst in the HER is significantly promoted by doping cobalt atoms. Recently, the Co–Mo–S phase, in which cobalt atoms decorate the edge positions of the MoS₂ slabs, has been identified as a co-catalytic phase in the Co-doped MoS₂ (Co-MoS_x) with low Co content. Here, we report the effect of the incorporation of cobalt atoms in the chemical state of the Co-MoS_x catalyst, which gives rise to the co-catalytic effect. Co-MoS_x catalysts with various Co contents were prepared on carbon fiber paper by a simple hydrothermal process. On the Co-MoS_x catalyst with high Co content (Co/Mo \approx 2.3), a dramatically higher catalytic activity was observed compared to that for the catalyst with low Co content (Co/Mo \approx 0.36). Furthermore, the co-catalytic phase in the Co-MoS_x catalyst with the high Co content was found not to be the Co–Mo–S phase but was identified as CoS₂ by Raman spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction, and transmission electron microscopy. It is believed that CoS₂ is an alternative choice to co-catalyze HER on MoS₂-based catalysts.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-466**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Simple digital microfluidic μ -dispenser on inkjet-printed, paper-based device

Haena Cheong, YUNPYO KIM, Oh-Sun Kwon^{*}, Kwanwoo Shin^{*}

Department of Chemistry, Sogang University, Korea

Digital microfluidics(DMF) has been merged as a liquid handling technique for micro-, pico- liter scaled biochemical experiments. In most experiments, controlling the liquid volume is a critical factor. To control the liquid volume precisely, we developed a simple μ -dispenser. The dispenser was composed of a reservoir electrode and an array of electrodes providing that a series of digital drops were generated out of each of reservoirs by electrowetting force. The droplet size varied as electrode size and applied voltage changed. So simple, easy and precise drop generation enabled the easy drop manipulation in a digital unit to replace the flow based in tedious numerous and spatial pipetting and vial lab-work. Printing method was used for fabrication of the patterned electrode of DMF chip plate which was required for electrowetting driven drop actuation actively as well as three elements, with conductive silver nanoparticle ink charged on an office inkjet printer. Additionally, the electronic plotter was used for mechanical cutting of Scotch tape for a dispenser well. As an application for this μ -dispenser, gold nano-rod synthesis was done on the DMF chip. by varying the growth condition by volume gold nanorods appeared with various aspect ratios. References[1]E. Samiei, M. Tabrizian, and M. Hoorfar, Lab on a Chip, 16, 2376 (2016)[2]H. Ko, J. Lee, Y. Kim, B. Lee, C.-H. Jung, J.-H. Choi, O.-S. Kwon, and K. Shin, Adv. Mater., 26, 2335 (2014).[3]R. Fobel, A. E. Kirby, A. H. C. Ng, R. R. Farnood, and A. R. Wheeler, Adv. Mater., 26, 2838 (2014).[4]N.R. Jana, L. Gearheart, and C.J. Murphy, The Journal of Physical Chemistry B 105.19 (2001)Keywords: Electrowetting, DMF, paper chip, inkjet printing, conductive ink, nanoparticle synthesis

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-467**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

The phase transition behavior of W-VO₂ near the metal-insulator transition point: a comparison of hydrothermally prepared granular powder cluster and thermally deposited film

Myeongsoon Lee, Don Kim*

Department of Chemistry, Pukyong National University, Korea

We report the physical properties of hydrothermally prepared W doped VO₂ cluster and thermally deposited W-doped VO₂ film. The precursor solution for the W-VO₂ samples was an aqueous mixture solution of ammonium vanadate (NH₄VO₃), oxalic acid (C₂H₂O₄) and ammonium paratungstate ((NH₄)₁₀H₂(W₂O₇)₆). The hydrothermal route results a mixture of vanadium oxides by the addition of W. In these sample, the metal to insulator transition (sudden change in T (K) vs. R (ohm) plot) was observed clearly at 330 K for pure VO₂ and shifted to 300 K by the addition of the W=0.03%. The change became unclear by the addition of the W. But no IR optical transition was observed in all the samples. On the other side, the thermal deposition route results high quality smart W-VO₂ films; sudden change in T (K) vs. R (ohm) plot and the transition temperature (T_{c-off}) shift from ~ 300 K to 250 K, and sudden change in T (K) vs. IR Transmittance (%)). We believe the formation of M-VO₂ phase is important to be a smart window, the W atom likes stabilized in the over oxidized vanadium oxides.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-468**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fabrication of graphitized carbon nanotubes decorated with gold&platinum nanoparticles by conversion of sucrose using AAO template

Myeongsoon Lee, Don Kim*

Department of Chemistry, Pukyong National University, Korea

We presented the fabrication of gold&platinum nanoparticles (AuNPs and PtNPs) attached carbon nanotubes (AuCNTs and PtCNTs). The preparation of AuCNTs and PtCNTs were performed through the carbonization of sucrose based on anodic aluminum oxide (AAO) template. The AAO template with ordered channel decorated with AuNPs and PtNPs were fabricated by a thermal decomposition of HAuCl_4 and H_2PtCl_6 . The size of AuNPs and PtNPs obtained from AAO template was confirmed by UV-Vis spectrum, TEM, HR-TEM images and XRD. The crystallinity of the CNT phase was confirmed by analyzing the G and D bands in their Raman spectra. We will discuss their chemical, electrical properties, and applications.

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Code: **MAT.P-469**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Enhanced Photovoltaic Performance of Perovskite Solar Cells Using Self-Assembled Molecules as Interfacial Layers

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¹*Chemistry, Kookmin University, Korea*

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Morphology and crystallinity of perovskite films are critical issue to achieve high performance perovskite solar cell. Herein, we study planar perovskite solar cell (PSCs) based on low-temperature ZnO as electron accepting layers (EALs) by utilizing self-assembled molecules (SAM) to achieve high efficiency PSCs. The SAMs is newly synthesized molecules, acted as excellent surface wetting control layers and also controlling the work function of ZnO-EALs. The insertion of SAMs improved the quality of perovskite films. In addition, it helps to make better energy level alignment for efficient charge extraction between the ZnO-EALs and perovskite active layers. As a results, our low-temperature ZnO based PSCs achieved high PCE of 18.8 % with improvement of all parameters such as VOC, JSC and FF, simultaneously. Keywords: perovskite solar cell, self-assembled molecules, interfacial layers, crystallinity, grain size

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Code: **MAT.P-470**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

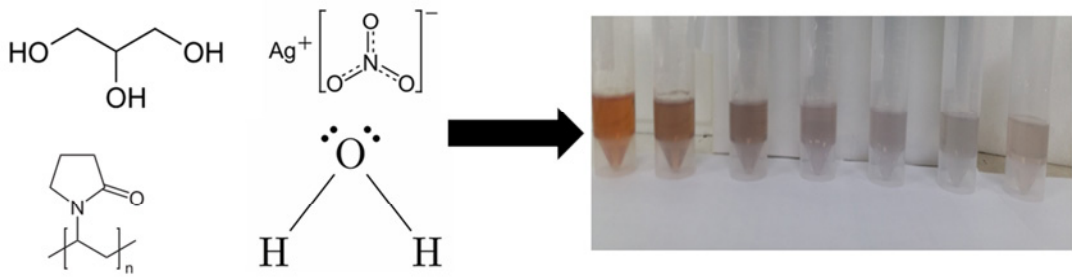
Complete Green Synthesis of Silver Nanoparticles using Glycerol and Synthetic Mechanism

JiSu Jeong, Jong Kuk Lim^{1,*}

Chosun University, Korea

¹*Department of Chemistry, Chosun University, Korea*

Since the first discovery for the synthesis of metal nanoparticles by Faraday, numerous methods to make nanoparticles of various shapes have been reported until now. In conventional method, usually harmful reducing agents (sodium borohydride et al.) are required to reduce metal ions or high temperature is needed to overcome activation energy. Researchers have been tried to develop eco-friendly synthetic method, and found that glycerol can be both solvent and reducing agent for making metal nanoparticles. Although glycerol is safe materials enough to be used as a sweetener in food, however, in glycerol-based synthetic method, alkaline condition is required, and which is not environmentally-friendly. Herein, we introduce complete green synthetic method to make silver nanoparticles where silver nanoparticles are synthesized in glycerol by glycerol at room temperature under neutral conditions.



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-471**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A comparative study of W, Nb and Mo-doped VO₂(M) nanoparticles prepared by the hydrothermal and post thermal transformation method

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Department of Chemistry, Pukyong National University, Korea

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VO₂(M) has recently redrawn much attention for energy-saving smart window applications because of thermochromic property due to phase transition. The phase transition temperature(T_c) is the key factor to make the application feasible. The pure VO₂(M) has a T_c of 69°C which is too high to be practical. The doping of high valent cations such as W⁶⁺, Nb⁵⁺ and Mo⁶⁺ has been known to be an effective method for decreasing T_c. Although there were several studies related to these doped VO₂(M), the results were not well established and conclusive depending on the physical state and preparation method. We have investigated the doped and codoped VO₂(M) nanoparticles prepared by the hydrothermal and post thermal transformation method where VO₂(B) was first prepared by hydrothermal reaction of V⁵⁺ precursor and reducing agent and thermally transformed to VO₂(M). In this study we are going to show the systematic and comparative study of the phase transition characteristics of VO₂(M) nanoparticles that are prepared by the hydrothermal and post thermal transformation method with doping W⁶⁺, Nb⁵⁺ and Mo⁶⁺ cations.

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Code: **MAT.P-472**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Hierarchical hydrophobic sponge for oil removal and catalytic degradation of toxic organics

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²*Seoul Women's University, Korea*

Soot is the natural byproduct of incomplete combustion, and candle soot is composed primarily of carbon element having hydrophobic nature. In this study, the superhydrophobic sponge (C/Ag-sponge) was prepared by hierarchical assembly of carbon nanoparticles generated from candle soot and silver nanoparticles. The hierarchical assembly was monitored by UV-vis-spectroscopy, and the structure of the C/Ag-sponge was characterized by field-emission scanning electron microscopy and transmission electron microscopy. The C/Ag-sponge has excellent oil separation efficiency with different densities such as hexane, chloroform and dichloroethane. In addition, the presence of silver nanoparticle on the sponge induced a good catalytic performance for the reduction of 4-nitrophenol after oil/water separation. We believe that the C/Ag coated sponge can be developed as one of promising candidates showing significant efficiency for water purification area.

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Code: **MAT.P-473**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

[Withdrawal] Charge Transfer Mechanism of Cs₂SnI₆-based Photoconversion Devices

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- Withdrawal -

KOREAN CHEMICAL SOCIETY

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-474**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Recycled fabrics coated with carbon nanoparticle for highly efficient oil/water separation

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²*Seoul Women's University, Korea*

Facial mask sheets are widely used as one of the most popular skin-care cosmetic items, and South Korea is the most leading country in terms of their production and export. Most of the mask sheets are composed of cosmetic emulsion or gels coated on cotton- or cellulose-based fabric sheet and disposable single-use products. Here, efficient recycle strategy of the wastes such as used-mask sheet and carbon soot was presented to fabricate superhydrophobic fabric filter for oil/water separation. The superhydrophobic filter was synthesized by a successive coating of positively-charged polyelectrolyte, negatively-charged carbon soot, and octadecyltrimethoxysilane (OTMS) on to used-mask sheet. The structure of resulting mask sheet was characterized by field-emission scanning electron microscopy and fourier-transform infrared spectroscopy. The superhydrophobic filter showed high oil/water separation efficiency (> 99%) for oils with various densities such as hexane, toluene, dichloroethane and chloroform. In addition, it showed an excellent separation performance in harsh environments such as highly acidic, alkaline, and salty environments, to deal with oil spills.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-475**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fabrication of ZnO-ZnS@polyaniline nano hybrid on FTO glass for enhanced Hydrogen generation

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Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea

Heterojunction structures are attracting lots of attention for enhancing the electron injection across the interface. ZnO-ZnS@polyaniline one-dimensional nano hybrid films are synthesized on conducting glass substrates in a controlled way, using a simple three-step electrochemical deposition, chemical sulfurization of ZnO nanowire array as reactive template and spin-coating technique. The Electrochemical measurements were performed using a 1 kW xenon lamp (Newport) with its infrared wavelengths filtered out by water, and wavelengths below 420 nm removed by an optical filter, enabling measurements under visible light. The light irradiance, measured by a thermopile detector, was 100 mW/cm². A monochromator (74,000, Newport) was used to investigate the monochromatic responses (for IPCE, applied bias photon to current efficiency (ABPE), and band gap energy measurements) of samples. 1 The as-prepared ZnO-ZnS@polyaniline one-dimensional nano hybrids are found to exhibit significantly an enhancement in the incident photon-to-electron conversion efficiency as compared to ZnO nanowire arrays. The observed enhancement in photoelectrochemical activity is attributed to the photosensitization effect of visible light responsive PANI. The special electron structure in the heterojunction helped to reduce the energy barrier height at the interface and enhanced the separation of photo-generated carriers. Thus, the photoelectrochemical performance and the dispersing stability of the composite photocatalysts in water were highly improved. Hence, our proposed structure is a promising candidate as a photoanode for solar energy-to-hydrogen conversion devices.*Corresponding Author: (BeeLyong Yang), (Kumoh National Institute of Technology, Korea), (blyang@kumoh.ac.kr)Reference: 1. Effect of seed layers on TiO₂ nanorod growth on FTO for solar hydrogen generation. Hyun Kim, Bee Lyong Yang. International Journal of Hydrogen Energy 40(2015) 5807-5814.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-476**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Band alignment offsets of PANI/ZnS/ZnO Heterojunctions

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Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea

ABSTRACT Energy band alignments at heterointerfaces play a crucial role in defining the functionality of semiconductor devices, yet the search for material combinations with suitable band alignments remains a challenge for numerous applications. The energy band alignment at the heterointerface between ZnO, ZnS and PANI was studied using photoelectron spectroscopy. We investigated band offsets at PANI/ZnS and ZnS/ZnO interfaces in a typical PANI/ZnS/ZnO heterojunction PEC cell by combining x-ray photoelectron spectroscopy and optical absorption spectroscopy. X-ray photoelectron spectroscopy and optical absorption spectroscopy measurements indicate that the conduction-band offsets at both PANI/ZnS and ZnS/ZnO interfaces show type-II alignment with values of 0.54 eV and 0.41 eV, respectively. Our results suggest that, although type-II alignment for PANI/ZnS heterojunction can form less of a barrier to electron transport across the interfaces, the narrowing of the interface barrier increases recombination of carriers.*Corresponding Author: (BeeLyong Yang), (Kumoh National Institute of Technology, Korea), (blyang@kumoh.ac.kr)

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Code: **MAT.P-477**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Photocatalytic reduction of carbon dioxide to methanol using Ag-loaded NiO/BaTiO₃/FTO

Bee Lyong Yang^{*}, Hyun Kim

Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea

As a cathode material for fuel generation from CO₂ reduction in a photoelectrochemical system, layered BaTiO₃/NiO films were developed and their surfaces were decorated with transition metals (i.e. Ag, Au, Cd, Cu, Pb, and Sn). Deposition of the transition metals effectively enhanced CO₂ conversion to fuel in terms of faradaic efficiency. In particular, Ag/NiO/BaTiO₃ demonstrated outstanding performance among the transition metals: for methanol yield production with high faradaic efficiency at -0.16 V (vs. SHE), which was a higher potential than standard redox potentials of methanol formation from CO₂. Moreover, electrochemical impedance spectroscopy (EIS) showed that the deposition of the transition metals onto BaTiO₃/NiO electrode effectively generated photo-induced electron-hole pairs under visible light irradiation. The reported system consisting of Barium Titanate and over-layer Nickel oxide loaded Ag NPs exhibits remarkable stability with time. *Corresponding Author: (BeeLyong Yang), (Kumoh National Institute of Technology, Korea), (blyang@kumoh.ac.kr)

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-478**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Tracking self assembly of nanoparticles using liquid phase electron microscopy

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¹*Seoul National University, Korea*

We present liquid cell TEM studies of self-assembly of nanoparticle by controlling concentrations of the initial solution and the types of nanoparticles and substrates. Through the in situ measurement, we understand the mechanisms of self-assembly driven by solvent drying at the single particle level. Our results showed that a solvent boundary affected nanoparticle motions and self-assembly processes in any conditions. The solvent boundary drove nanoparticles to form 2D assembly mainly through two pathways, lateral dragging and vertical pressing.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-479**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Relationship Between Particle Size Distribution/Particle Shape and Optical Properties of Gold Nanoparticles

MISUN PARK

Headquarters for Administration, Dong-II SHIMADZU Corp., Korea

Metallic nanoparticles are known for their specific properties and are employed in a wide range of fields. In particular, gold nanoparticles are attracting attention in fields such as bioimaging and high-density data storage media because its optical properties change according to particle size and shape. This article presents the findings of using the UV-2700 UV-VIS spectrophotometer to measure changes in optical properties according to differences in the size and shape of gold nanoparticles, the SALD-7500nano nano particle size analyzer to examine particle size distribution, and the SPM- 9700HT scanning probe microscope to examine particle shape.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-480**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Strain sensor with organic single crystal nanowires by direct printing

YOONKYOUNG PARK, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

Charge transport properties of organic semiconductors critically depend on their molecular packing structures. Controlling the charge transport by varying the molecular packing and understanding their structure–property correlations are essential for developing high-performance organic electronic devices. Here, we demonstrate that the charge carrier mobility in organic single-crystal nanowires can be modulated with respect to the intermolecular center-to-center distance by applying uniaxial strain to the cofacially stacked crystals. Monotonic changes in charge carrier mobility (from 0.0196 to 19.6 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ for 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-PEN)) were observed under a wide range of strains from -16.7% (compressive) to 16.7% (tensile). Furthermore, the measured values of charge carrier mobility were in good agreement with theoretical calculations based on charge localized hopping theory. These results provide a definitive relationship between intermolecular packing arrangement and charge transports, which enables a huge improvement in charge carrier mobility for organic single-crystal materials.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-481**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

A non-destructive n-doping method for graphene with precise control of electric properties via atomic layer deposition

Jinwon Jung, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

The graphene, a single atomic sheet of graphite, has attracted many researchers attention in these days because of its unique conical energy dispersion relation at the charge neutrality (Dirac) point in the electronic band structure. From that, graphene has superior intrinsic mobility compared to other semiconductors. Optical transparency and flexibility of graphene are also crucial properties for new era in semiconductor industry. However, for more diverse application of graphene devices, precise control of the carrier type and carrier concentration in graphene also plays an important role in the device performance as well as the device design. So, herein, we present atomic layer deposition (ALD) of zinc oxide (ZnO) on graphene as a non-destructive n-doping method that enables precise control of electrical properties of graphene through fine control over the ZnO film thickness and ensures high air stability of the graphene devices from complete and uniform surface coverage with air-stable ZnO thin films. By using 4-mercaptophenol as a reactive organic molecular layer. We can deposit uniform ZnO thin films of good quality with a low density of pinholes on graphene. Through π - π stacking between chemically inert graphene and 4-mercaptophenol, conformal deposition of ZnO on graphene was enabled without any damage of graphene. The electron mobility of graphene TFT significantly enhanced by the n-doping effect compared to the pristine graphene. This ZnO doping method by atomic layer deposition can be applicable to large scale array of CVD graphene TFT and is well suitable for non-destructive fine-tunable doping of two dimensional materials including not only graphene but also other 2D materials.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-482**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Ultrahigh barrier performance of Organic-inorganic nanolaminated thin films

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Organic light-emitting diodes (OLEDs) have emerged as a potent candidate for next-generation displays due to their multiple advantages in terms of color reproduction, wide viewing angles, fast response times, and low-voltage operation. However, the metal electrodes and organic materials currently being used in OLEDs are very sensitive to moisture and air, limiting their lifespan. For commercial applications, the water-vapor transmission rate (WVTR) of approximately 10^{-6} g m⁻² day⁻¹ requirement must be achieved for effective encapsulation. This work presents a novel barrier thin film based on an organic-inorganic nanolaminate, which consists of alternating nanolayers of self-assembled organic layers (SAOLs) and Al₂O₃. The SAOLs- Al₂O₃ nanolaminated films were deposited using a combination of molecular layer deposition and atomic layer deposition techniques at 80 °C. Modulation of the relative thickness ratio of the SAOLs and Al₂O₃ enabled control over the elastic modulus and stress in the films. Furthermore, the SAOLs- Al₂O₃ thin film achieved a high degree of mechanical flexibility, excellent transmittance (> 95%), and an ultralow WVTR (2.99×10^{-7} g m⁻² day⁻¹), which represents one of the lowest permeability levels ever achieved by thin film encapsulation. On the basis of its outstanding barrier properties with high flexibility and transparency, the nanolaminated film was applied to a commercial OLEDs panel as a gas-diffusion barrier film. The results showed defect propagation could be significantly inhibited by incorporating the SAOLs layers, which enhanced the durability of the panel.

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Code: **MAT.P-483**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Highly sensitive ammonia gas sensor based on single-crystal Poly(3-hexyl thiophene) (P3HT) organic field effect transistor

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A highly sensitive Organic field-effect transistor (OFET)-based sensor for ammonia in the range of 0.01 to 25 ppm was developed. The sensor was fabricated by employing an array of single-crystal Poly(3-hexyl thiophene) (P3HT) nanowires as the organic semiconductor (OSC) layer of an OFET with a top-contact geometry. The electrical characteristics (field-effect mobility, on/off current ratio) of the single-crystal P3HT nanowire OFET were about two orders of magnitude larger than those of the P3HT thin film OFET with the same geometry. The P3HT nanowire OFET showed excellent sensitivity to ammonia, about 3 times higher than that of the P3HT thin film OFET at 25 ppm ammonia. The ammonia response of the OFET was reversible and was not affected by changes in humidity. The high ammonia sensitivity of the P3HT nanowire OFET is believed to result from the single crystal nature and high surface/volume ratio of the P3HT nanowire used in the OSC layer.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-484**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

High conductive ZnO thin film deposition for Atomic Layer Deposition in in situ UV illumination

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Zinc Oxide (ZnO) thin film received attention for transparent conducting electrodes. Also, ZnO is widely used in various optoelectronic devices for transparent electronics and sustainable energy generation, such as LEDs, and solar cells. Transparent conductive oxides having a wide band gap to transmit the visible spectrum of light. However, ZnO does not have enough conductivity to use the applications. Doping process is essential to increase the conductivity. Despite the higher concentration of dopant leads to enhance the carrier concentration, while transmission does not. The conductivity of ZnO film can also be enhanced by improving the carrier mobility. It is known that the negatively charged oxygen species at grain boundaries act as trapping centers that suppress electron transfer. Thus, the grain boundary defects decrease carrier mobility. Passivation of grain boundary by thermal treatment of ZnO in reducing atmosphere such as in hydrogen can simply reduce the potential barrier for electron transfer at grain boundaries.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-485**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Synthesis, cytotoxicity, and photochemical properties of rhodamine based fluorescent probes

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Rhodamine derivatives are heterocyclic compound, related to the fluorescent probe having a profound application in the field of biotechnology. Herein, we present rhodamine based fluorescent probes synthesized from rhodamine B (Probe 1) and rhodamine 6G (Probe 2). The structure of the synthesized Probes 1 and 2 were confirmed using ¹H NMR. Further, photo physical properties viz. absorption spectroscopy, fluorescence spectroscopy and fluorescence lifetime were measured and compared for both the probes under identical conditions. These comparable data give a possibility to discuss the idea about mechanism which controls the fluorescence properties of probes. The data also showed that a gradual change in the molecular chemical structure of the probe alters the solvent environment and produces a change in fluorescent intensity as a sensory signal. The changes in fluorescence lifetime and quantum yield with the parent compounds is because of change in solvent polarity and also due to the rigidity of the alkyl groups on -N atoms in molecular structure. Further to extend the comparison between the probes, the cell imaging and cellular toxicity studies were performed. The results obtained in experiments suggest that synthesized probes show a great promise for application in field of cellular imaging or biotechnology.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **MAT.P-486**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Development of Novel Metal Composite Catalysts for Dehydrogenation of Formic Acid

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As a clean and sustainable energy carrier, hydrogen has attracted significant attention. Despite of its potentials, hydrogen production, storage, and utilization still possess technical limitations for widely applicable hydrogen-based energy. To achieve hydrogen economy in a near future, hydrogen storage issue should be resolved particularly. Numerous material candidates for hydrogen storage were proposed to address this issue. Especially, liquid chemicals are advantageous owing to the high volumetric energy storage densities with safe and economical transportation. One of the promising materials is formic acid (FA), which releases H₂ even at ambient condition and can be easily transported into a desired site. However, decomposition of FA can be proceeded via two pathways to give hydrogen and carbon dioxide as a product (HCOOH→H₂+CO₂, dehydrogenation) or to release carbon monoxide (HCOOH→H₂O+CO, dehydration) which is detrimental to fuel cell applications. Therefore, it is required to develop highly selective and active catalysts for FA dehydrogenation. We present here the preparation, characterization, and H₂-release properties of novel metal and composite catalysts and their catalytic activities toward FA dehydrogenation.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facile synthesis of Nanoporous Gold Nano-Shell structure using plasma treatment

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A nanoporous gold nanoparticle (NPGNP) is a plasmonic nanoporous structure with advantages of large surface area and multiple hot-spots in a small nanoscale overall size. Due to strong enhancement of electromagnetic field at multiple hot-spots by localized surface plasmon resonance (LSPR), NPGNP can be promising for the sensing application such as surface-enhanced Raman scattering (SERS) to detect small amount of target materials. The plasmonic property of NPGNP can be tuned by its structural parameters. Here, we propose a new way to synthesize a nanoporous gold nano-shell (NPGNS) structure with various overall size and ligament size by using a simple air-plasma treatment, and demonstrate its application for SERS.

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Code: **MAT.P-488**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

PdNi Metal Alloy Nanoparticles as Efficient catalyst for Formic Acid Dehydrogenation

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¹Fuel Cell Research Center, Korea Institute of Science and Technology, Korea

As the sustainable and renewable energy source, hydrogen has been received increasing attention. To realize the hydrogen economy, hydrogen production, storage, and transportation are the key factors that need to be resolved. Among these technologies, a safe and economic hydrogen storage technology is particularly demanded for the flexible energy utilization. In this context, formic acid (FA) has been considered as a potential liquid hydrogen carrier because it has high volumetric hydrogen storage density (53 g/L) with economically viable transportability. For formic acid to be useful as a hydrogen carrier, it is necessary to develop highly active and selective catalysts. To achieve better catalytic activity with higher economic feasibility, we made an attempt to synthesize alloyed metal nanoparticles in combination of noble metals with relatively cheap metal components to achieve enhanced catalytic formic acid dehydrogenation over catalyst surfaces by modifying the surface electronic structure of metal nanoparticles. Our results showed that both activity and selectivity of FA dehydrogenation over PdM catalyst were found to be highly dependent on added temperature and metals (M).

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Code: **MAT.P-489**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Aligned perovskite crystal arrays and its optoelectronic applications

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Organometallic perovskites $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($X=\text{Cl, Br, I}$) have received great attention because of their excellent photoelectrical properties as well as their low-cost device fabrication process. The exceptional light-harvesting and superior carrier transport properties lead to the advanced performances of these materials in various applications such as Solar cells, LASERS, LEDs, and photodetectors. Typically, one of the most important factor to decide the efficiency of these applications is the quality of the crystal. Even though, optoelectronic devices are composed of polycrystalline thin film in general, not a single crystalline form which has longer carrier diffusion length and higher mobility. For these reasons, perovskite single crystals have potential to elicit an optimized device efficiency. In this study, we fabricate the aligned perovskite crystal arrays in thin film form and characterize the crystallography of the perovskite thin film by X-ray diffraction (XRD) and selected area electron diffraction (SAED). Also, the morphology of perovskite crystals was observed using scanning electron microscopy (SEM). Furthermore, the perovskite patterned thin films are applied in lateral solar cell application. The average efficiency of the perovskite lateral solar cell in low light intensity is over 4%, which are the world-top efficiency in lateral perovskite solar cell field as far. From this work, the probability of the aligned perovskite single crystal array is demonstrated.

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Code: **MAT.P-490**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Surface Design of Separators for Oil/Water Separation with High Separation Capacity and Mechanical Stability

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A convection heat treatment that can replace existing chemical oxidation methods was developed for the preparation of hierarchically oxidized Cu meshes with various surface morphologies, representing a very simple and green route that does not involve toxic chemicals. Three types of Cu meshes [bumpy-like (BL) and short and long needle-like (NL) structures] exhibited similar separation efficiencies of 95–99% over 20 separation cycles, as indicated by their similar water contact angles (WCAs; 147–150°). However, these Cu meshes exhibited different flux behaviors. Excessively rough and excessively smooth surfaces of the Cu mesh resulted in increased resistance to flow and to a decrease of the penetration of oil. A surface with intermediate smoothness, such as the BL-Cu mesh, was necessary for high flux over a broad range of oil viscosities. Furthermore, a less rough surface was more suitable for the separation of highly viscous oil. Computational fluid dynamics (CFD) simulations were carried out to support our experimental results. The BL-Cu meshes also showed outstanding mechanical stability because of their low resistance to the flow of fluids.

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Code: **MAT.P-491**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Magnetic Amphiprotic Catalysts and Separators Coping with Environmental Issues

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Abstract Amphiprotic catalysts have recently gained increased interest particularly regarding applications in oil/water separation and pollutant purification. Many industries produce and emit oil/water mixtures containing aqueous and non-aqueous pollutants as wastewater. The amphiprotic catalysts reported thus far have used separated processes for oil/water separation and pollutant purification, which is not suitable for industrial applications requiring in-situ and continuous processes for oil/water separation and pollutant purification. Moreover, to the best of our knowledge, amphiprotic catalysts that can freely move between two phases, such as oil and water, to perform functions in each phase, such as the decomposition of aqueous and non-aqueous pollutants, have not been reported. Here, we report a novel approach-based magnetic amphiprotic catalyst (MAC) that can freely move between oil and water to perform functions in each phase, enabling the in-situ and continuous processes for oil/water separation and the decomposition of aqueous and non-aqueous pollutants in both phases. References [1] Li, S.; Jiao, X.; Yang, H. Hydrophobic core/hydrophilic shell structured mesoporous silica nanospheres: enhanced adsorption of organic compounds from water. *Langmuir* 2013, 29, 1228-1237. [2] Lee, Y. S.; Bae, J. Y.; Koo, H. Y.; Choi, W. S. A remote-controlled generation of gold@ polydopamine (core@shell) nanoparticles via physical-chemical stimuli of polydopamine/gold composites. *Sci. Rep.* 2016, 6, 22650.

Conference Date: October 18~20, 2017

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Code: **MAT.P-492**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Self-floating and Submerging Sponge Adsorbents for Environmental remediation

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Water pollution by heavy metals and organic dyes has become a serious environment issue. Diverse technologies have been reported to eliminate these pollutants. Among these methods, nanoadsorbents are of particular interest in wastewater treatment because of their high surface-to-volume ratio, which leads to a higher uptake capacity. However, most of the reported nanoadsorbents are flow type, which are very vulnerable to leakage in the process of separation because they are dispersed or precipitated. It has been recently reported that the unintended leakage of nanomaterials into the environment can cause a significant threat to the environment and public health. Here, we report a janus sponge composite that can be partially floated/submerged on/in the water to perform efficient adsorption of pollutants without leakage of adsorbents.

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Code: **MAT.P-493**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Al₂O₃ Thin Film Preparation by UV light enhanced Atomic Layer Deposition

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We have performed Al₂O₃ thin films deposition at room temperature by UV-enhanced atomic layer deposition on poly(ethylene terephthalate) (PET) substrates. We have used trimethylaluminum (TMA) for metal source and H₂O for oxygen source as precursors with UV irradiation. The atomic layer deposition depends on alternate pulsing of the precursor gases onto the substrate surface followed by chemisorption of the precursors onto surface. In general cases, the surface reactions of the atomic layer deposition are not completed at low temperature. In this experiment, the reactions were found to be self-limited surface reaction and complementary enough to yield uniform Al₂O₃ thin films by using UV irradiation at room temperature. The UV light was very efficient to get the high quality Al₂O₃ thin films without any defect on polymer substrate. The thickness, density, morphology and electrical property of the Al₂O₃ thin films were measured by AFM, XRR, ellipsometry, and C-V measurement.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Interface engineering for high-performance organic-inorganic hybrid Sb₂S₃ solar cell by atomic layer infiltration

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The Sun provides a sustainable, reliable and long-term supply of energy, in contrast to conventional resources such as coal and fossil fuels, and can therefore help to solve the growing global need for energy. Above all, Si solar cell is the most widely used as energy source due to its high efficiency and confirmed stability. But, Si solar cells have a disadvantages; expensive manufacturing cost and limitation of application to flexible or transparent devices. So other types of solar cells are also being studied, Sb₂S₃ solar cell is a prospective substitution for next generation solar cells overcoming the above disadvantage of Si solar cell. The biggest problem of commercialization of Sb₂S₃ solar cell is lower efficiency than Si solar cells. To solve this obstacle, previous studies about interfacial engineering have been proceeding using various organic, inorganic materials. Here, we introduced new application; organic-inorganic hybrid material nickel-4-mercaptophenol (Ni-4MP), as an interfacial engineering material into Sb₂S₃-hole transport material (HTM) interface. Ni-4MP thin film is deposited using atomic layer deposition (ALD) method. For infiltrate precursors into FTO/mp-TiO₂/Sb₂S₃ structure, exposing procedure is added. The reference cell structure is FTO/mp-TiO₂/Sb₂S₃/P3HT/Au. We measured the photo conversion efficiency using solar simulator with source-meter for comparing two samples. And then we observed impedance measurement with variation of voltage for confirming the effect of Ni-4MP on Sb₂S₃ solar cell. As a result, these measurements proved that electron life-time is increasing by inserting Ni-4MP as interfacial engineering material.

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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Facile synthesis of Se/graphene nanocomposites for energy storage application

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As a novel two-dimensional carbon material, graphene has drawn increasing attention due to its outstanding optical, chemical, physical properties and promising applications in electronics, energy storage and photovoltaics. Selenium is an alternating electrode material due to the chemical properties similar to sulfur, but electric conductivity is approximately 20 orders of magnitude greater than that of sulfur. The high electric conductivity enables better utilization of selenium active materials and fast electrochemical reactions. In this study, the Se/graphene nanocomposites were hydrothermally treated and hybridized with Se nanoparticles and graphene oxides. Physicochemical properties of the synthesized Se/graphene nanocomposites were characterized by XRD, FT-IR, SEM, TEM, RAMAN and XANES analysis. Electrochemical tests indicate that nanocomposites could be used as a good anode material for the development of sodium ion batteries with excellent performance.

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Area: Material Chemistry

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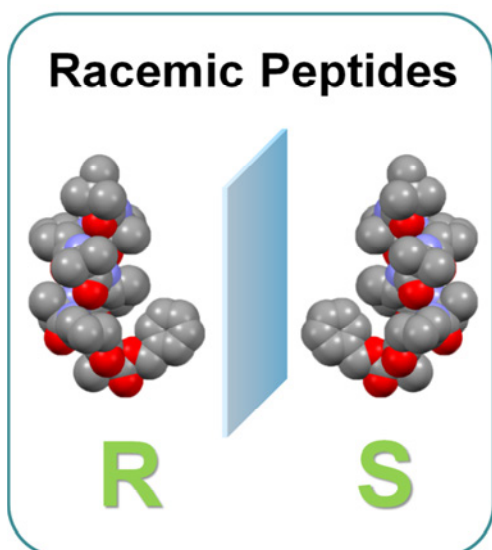
Morphological and Structural Features of Foldectures by the Self-Assembly of Racemic Foldamers

Jae-Hoon Eom, Jintaek Gong¹, Hee-Seung Lee^{*}

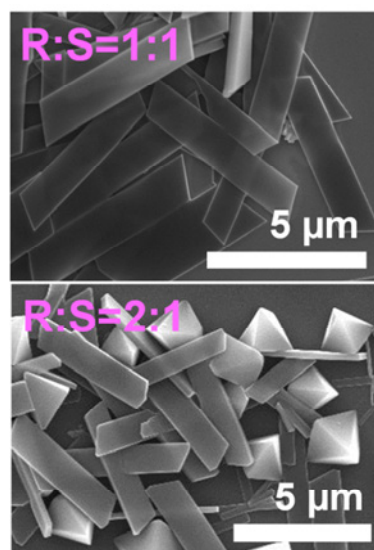
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Self-assembly of biomaterials have attracted enormous attention due to their potential applications in catalysis, biomedicine and nanoelectronics. We have recently reported that peptide foldamers with well-defined secondary structures self-assembled in aqueous solution to provide a series of highly homogeneous and unique 3D morphologies, named foldectures. Because they possess highly crystalline nature, the molecular packing modes of foldectures could be analyzed by powder X-ray diffraction analysis. For these studies, we prepared foldamer building blocks from enantiomerically pure beta-amino acid monomers, as this is a necessary criterion for intramolecular folding in most secondary structures of peptides. On the other hand, self-assembly using racemic peptide building blocks has rarely been attempted presumably because it may provide complex aggregates or assemblies with ill-defined morphologies. Interestingly, however, it has been reported that racemic proteins or DNAs showed higher tendency to crystallize than enantiomerically pure forms because of the propensity for enantiomers to act as “tailor-made” impurities that initiate crystallization. Herein we report that parallelogram plate shaped foldectures are obtained from an equimolar mixture of enantiomeric foldamer, while trigonal bipyramid shaped foldectures are formed from pure enantiomeric foldamer.



Self-Assembly



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Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

UV enhancement of electrical and optical properties from Al-doped ZnO films prepared by atomic layer deposition at low temperature

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Doped ZnO was commonly used for the transparent conducting electrodes, but it was not suitable for flexible application so far, because the high fabrication temperature was essential to achieve good electrical properties. In this study, ZnO/Al₂O₃ (Al-doped ZnO) multi layers were fabricated by alternating Atomic layer deposition (ALD) on PET substrate at 130 °C using diethylzinc (DEZ), trimethylaluminum (TMA) and deionized water with additional ultra-violet (UV) exposure. The growth rate, electrical and optical properties of the multi layers were studied with a variety of cycle ratio of ZnO and Al₂O₃ sub layers. The ZnO/Al₂O₃ multi layers deposited at 120 °C has low conductivity. However, after few minutes of UV light exposure, the films show high conductivity. The conductivity can be controlled to positive direction by increasing the UV exposure time. Furthermore, the film showed high transparency(80%) and high stability against the degradation of the electrical conductivity.

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Code: **MAT.P-498**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Wafer scale well-connected CVD-grown graphene grains by using selective atomic layer deposition of ZnO

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Recently, graphene has attracted much attention due to its outstanding properties such as ultrahigh mobility, mechanical strength, thermal conductivity and transparency. Therefore, nearly a decade of graphene research has promised potential applications including longer-lasting batteries, more efficient solar cells, corrosion prevention, circuit boards, display panels. For commercial applications, large-scale CVD-grown polycrystalline preparation of high quality graphene is a requirement in next generation electronics, optoelectronics, and chemical and biosensors. However, large scale CVD-grown graphene containing numerous grain boundaries that would effectively scatter charge carriers, thereby forming highly resistive barriers and adversely affect to restrict electronic properties of graphene in general and especially carrier mobility in particular. In this research, large-scale CVD-grown graphene is enhanced electronic transport properties by selective deposition of hexagonal ZnO on defect-rich reactive and grain boundaries using atomic layer deposition (ALD) technique. The CVD graphene is improved significantly inter-grain mobility with only a negligible change in the free carrier density. An enhanced connectivity between graphene grains was obtained showing an excellent mobility of graphene thin film transistor. Furthermore, selective deposition of ZnO on CVD graphene can be successfully applied into wafer-scale arrays on 4-inch Si and polymer substrates, revealing remarkable device-to-device uniformity. In brief, we report that the large-scale well-connected graphene is useful not only for the study of electronic properties of CVD graphene but also for improving other properties of CVD graphene, such as thermal conductivity, mechanical strength, and gas permeability.

120th KCS General Meeting & Exhibition

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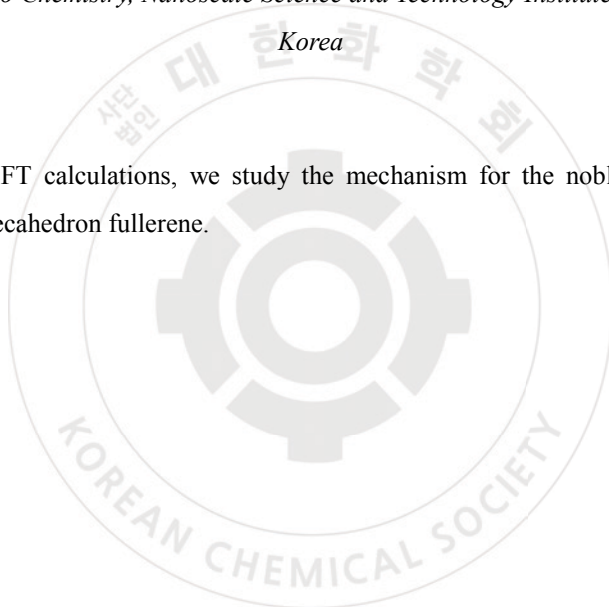
Type: Poster Presentation, Time: THU 11:00~12:30

Metastable C₂₀ Cage Structures

Kee Hag. Lee^{*}, Yong Jae Cho, Kayoung Kook, Minjeong Jang

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Korea*

By using the hybrid DFT calculations, we study the mechanism for the noble metastable C₂₀ cages obtained from C₂₀ dodecahedron fullerene.



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Code: **MAT.P-500**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Formation of highly transparent reduced graphene oxide films by Langmuir-blodgett technique

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¹*Center for Advanced Instrumentation, Korea Research Institute of Standards and Science, Korea*

Graphene has been extensively applied in various research fields due to its excellent physical and electrical properties. Researcher have developed different methods such as electro-spray, bar-coating and painting to form the graphene films which exhibit good electrical properties. However, the films prepared by these conventional methods show low optical properties. To solve this problem, we utilized a Langmuir-Blodgett (LB) technique. Firstly, the graphene oxide films were transferred to different substrates. Then, the reduction of graphene oxide film was done by hydrazine gas. Finally, the reduced graphene oxide films were achieved with high transmittance. We varied the experiment conditions and investigated the optical properties.

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Code: **MAT.P-501**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Fabrication and Characterization of New Organic-Inorganic Hybrid Thin Films

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New materials are required for the next generation devices. One of the ways to fabricate new materials is the hybridization of existing materials having different properties. The hybrid materials mixed by organic and inorganic components are expected to have combined properties both of inorganic parts, such as stability and high electrical or optical performance and organic parts, such as flexibility and functionality. Furthermore, the hybrid materials are expected to have synergic effects which are not shown in just one component. Herein, we fabricated new types of organic-inorganic hybrid thin films by molecular layer deposition. The hybrid thin films were made by sequential surface reactions of metal alkyls and bifunctional monomers. Diethyl zinc and 2,4-hexadiyne-1,6-diol are used as an inorganic precursor and an organic precursor, respectively, in order to fabricate poly(zinc diacetylene). Some methods are used to characterize the microstructure and compositions of the hybrid films such as Raman, XPS and TEM analysis. And, the electric and optical properties were analyzed by a TFT fabrication and photoluminescence spectroscopy, respectively. The high performance of TFTs, on/off ratio of over 10^7 and saturation electron mobility of over $10 \text{ cm}^2/\text{V}\cdot\text{s}$, and the low temperature process indicate the possible use of the hybrid films to flexible devices

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Code: **MAT.P-502**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

Correlation of lattice strain with HER catalytic activity of Ni₂ P nanowires

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Ni₂ P nanowire 는 촉매 분야에서 높은 HER 활성도를 갖는 물질로써 각광받고 있다. 이러한 촉매활성도를 갖고 있는 물질에서 촉매반응이 나타나는 방향에 대해 연구는 대부분 계산에 의존해 왔으며, 이에 대한 TEM 내에서의 직접적인 분석은 HRTEM image 분석과 EDS 성분분석으로 극히 제한적이다. 본 연구에서는 기존의 연구와는 다른 Topspin 이라는 고도분석을 도입하였다. 이 분석방법은 TEM 내에서 2nm 의 나노회절패턴과 전자빔의 세차회절 방법을 동시에 사용하여 격자변형량을 측정함으로써, Ni₂ P nanowire 에서의 HER 촉매활성 이후에 나타난 격자변형량에 대해 측정 및 해석하였다. 이 방법은 해당영역에 대하여 수만장의 나노 회절패턴을 매트릭스 형태로 측정하여 분석하기 때문에 기존의 HRTEM 이미지와 SAD 패턴의 단점이었던 해석의 모호성을 제거 함과 동시에 높은 촉매활성도가 나타나는 면의 격자변형량을 분석할 수 있었다. 그 결과 Ni₂ P nanowire 에서 HER 반응후에 촉매활성도가 높은 영역에 대한 strain mapping 을 얻었으며, 001 면에서의 strain 변화가 두드러지게 나타난 것을 확인하였다.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **MAT.P-503**

Area: Material Chemistry

Type: Poster Presentation, Time: THU 11:00~12:30

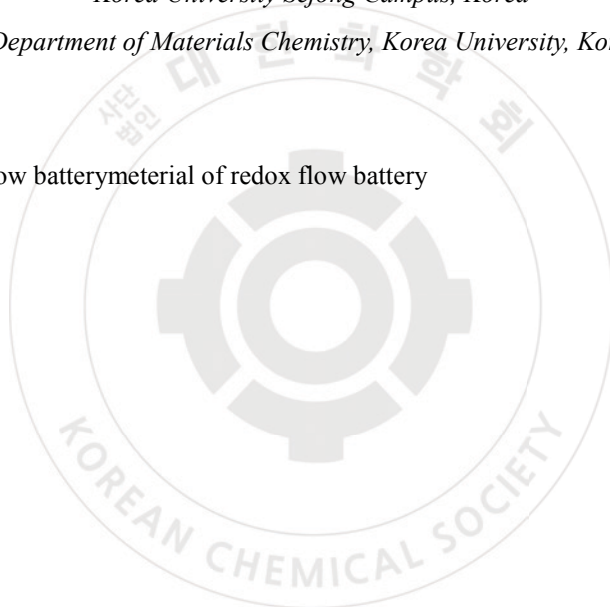
Redox flow battery

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introduction of redox flow battery material of redox flow battery



Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-449**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Sonochemical Preparation and characterization of Amorphous earth-abundant metal oxide Nanoparticles as Electrocatalysts for Oxygen Evolution Reaction

Ah-Hyeon Park, Hyun-Uk Park, jong un jung, Young-Uk Kwon*

Department of Chemistry, Sungkyunkwan University, Korea

In the for electrical energy storage system, the metal-air battery with high theoretical specific energy is attractive technology that overcoming the limit of Li-ion battery such as low driving range and energy density. However, due to the limitations of high operating voltage and low cycle life, it is necessary to use oxygen evolution reaction (OER) catalyst to increase the energy efficiency. IrO_x and RuO_x are commercial OER catalyst but its element scarcity and high cost hindered the commercialization. Therefore, earth-abundant metal oxide compound is emerging as an alternative. Herein, we present the sonochemical synthesis that synthesizes a non-precious metal compound with binary and ternary metal system and their electrochemical performance in alkaline electrolyte solutions. We prepared a binary metal compound with 1:1 ratio using 1st transition metal precursor and measured OER electrocatalytic performance and durability through the electrochemical interaction between metal. Among them, Sample that includes Fe, Co, and Ni showed excellent catalytic activity and Ni-Fe oxide compound showed superior OER catalytic activity and durability. In case of controlling the metal composition regarding the Ni-Fe and Fe-Co system showing the best catalytic activity, while Fe-Co system showed similar activity without reference to metal ratio, Ni-Fe system exhibited Volcano-type trend according to the metal ratio and $\text{Ni}_{70}\text{Fe}_{30}$ sample showed the best catalytic activity. Based on our results, we demonstrated that the electronic structural change by metal-metal interaction affected to electrochemical performance and expected to improve its electrochemical catalytic performance.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-450**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

One-pot Synthesis of PdFePt Ternary Electrocatalyst with Synergetic Effect and Their Electrocatalytic Properties for Oxygen Reduction Reaction

Hyun-Uk Park, Wenjuan Shi, Ah-Hyeon Park, Jongun Jung, Young-Uk Kwon *

Department of Chemistry, Sungkyunkwan University, Korea

In this work, we have studied synergetic effect of PdFePt nanoparticles (NPs) supported on carbon support (PdFePt/C) along with different Pd precursors (Pd(acac)₂ and PdO) and investigated their electrocatalytic performance for oxygen reduction reaction (ORR). PdFePt/C_Pd(acac)₂ and PdFePt/C_PdO samples showed 4.5 and 2.8 nm sized PdFePt NPs respectively, and were synthesized by a one-step ultrasound-assisted polyol synthesis (UPS). For the preparation of PdFePt/C samples, Pt(acac)₂, Fe(acac)₃, Pd(acac)₂ (or PdO) and carbon support were dispersed in ethylene glycol and irradiated by ultrasound for 3 h. Based on the structural characterization, we found that PdFePt/C_Pd(acac)₂ sample have wide particle size distribution because of such big nanoparticles, whereas PdFePt/C_PdO sample show relatively well-dispersed and uniform sized PdFePt NPs on carbon support. It assumed that there might be difference pathway for particle growth during the synthetic process arose from different Pd precursors. Electrocatalytic properties of samples were investigated by rotating disk electrode (RDE) measurement. Compared with commercial Pt/C, PdFePt_Pd(acac)₂ and PdFePt/C_PdO samples showed the enhanced ORR activity and durability in acid media. In conclusion, we observed that the synergetic effect of PdFePt ternary electrocatalyst along with types of Pd precursors and it can play a important role in electrocatalytic performance and durability.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-451**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile sonochemical synthesis of PdCu alloy as highly active electrocatalysts for methanol oxidation reaction

WEN JUAN SHI, Hyun-Uk Park, Ah-Hyeon Park, Jongun Jung, Young-Uk Kwon*

Department of Chemistry, Sungkyunkwan University, Korea

The high performance of Pd-based bimetallic nanocatalysts has the potential to replace Pt-containing catalysts for the direct methanol fuel cells. Conventionally, bimetallic particles are obtained through the annealing of nanoparticles. However, this research demonstrates a simple sonochemical synthesis method to fabricate the palladium-copper alloy (PdCu alloy). Our approaches involve the reduction of Pd and Cu using ethylene glycol as the solvent and reduction agent and Ketjen Black as the carbon support. The crystal structures, alloy compositions and morphologies of catalysts are determined by X-ray diffraction (XRD), energy dispersive spectrometer (EDS) and transmission electron microscopy (TEM), respectively. XRD patterns of samples show the formation of the face-centered cubic crystalline Pd on the carbon support for the PdCu/C catalysts. TEM images show that the PdCu alloy nanoparticles (NPs) are well-dispersed on the carbon support, and the sizes of the nanoparticles can be controlled by adjusting the composition of the raw mixtures. Moreover, EDS results indicate the uniform compositions of Cu and Pd atom. The electrocatalytic properties of PdCu alloys have been investigated by rotating disk electrode (RDE). The PdCu alloy with atomic ratio of 30.8% Cu exhibits a higher electrocatalytic activity and lower onset potential in 0.1 M KOH electrolyte containing 1 M methanol solution.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-452**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Advanced separator of high performance to maximize the effect of the soluble catalyst for Li-O₂ batteries

seonhwa lee

Department of Energy Engineering, Hanyang University, Korea

Li-O₂ batteries have a major obstacle regarding the large overpotential upon charging that results from the low conductivity of the discharge product. Thus, various re(RMs) have been widely studied to reduce the overpotential upon the charging process; this should help promote the oxidation of Li₂O₂. However, since RMs degrade the Li metal anode through a parasitic reaction between the RM and the Li metal, a solution is needed to rectify this phenomenon. Here, we propose an effective method to prevent the migration of the RM toward the anode side of the lithium metal by using a modified separator with a negatively charged polymer. When DMPZ (5,10-dihydro-5,10-dimethylphenazine) is used as the RM, we find that the modified separator suppressed the migration of DMPZ toward the counter electrode of the Li metal anode; this is investigated by a visual redox couple diffusion test, morphological investigation, and X-ray diffraction study. This advanced separator effectively maximizes the catalytic activity of the redox mediator. Li-O₂ batteries using both a high concentrated DMPZ and the modified separator exhibit improved performances and maintain 90% of the roundtrip efficiency up to the 20th cycle.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-453**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Pouch Type Cells for Large-Scale Li-air batteries

WONJIN KWAK

Department of Energy Engineering, Hanyang University, Korea

Li-air batteries are considered as candidates for next-generation battery systems in place of conventional Li-ion batteries for advanced applications such as electric vehicles (EV).¹⁻³ However, low energy efficiency, poor cycle life and Li-metal safety issues make the use of Li-air batteries yet impractical. In addition, actual cell capacities are very low and, since only small-scale electrodes are currently tested, it is hard to predict the properties of large-size electrodes and cells, thus evaluating and judging real practical challenges related to this battery technology. Here, we report on fabrication, operation and evaluation of pouch-type Li-air cells using $3 \times 5 \text{ cm}^2$ sized electrodes, in which we intend deal with higher capacity (mAh) of the electrodes, compared to most previous studies in the field. With the relatively large-sized cells, operating at high current density and capacity, we could recognize some remarkable problems that may not be significant in small cells. In relatively large cells as those explored in this work issues related to non-uniform current distribution, mechanical and electronic integrity of electrodes are much more influencing compared to small cells. Hence, problems such as lithium dendrites formation and non-uniform deposition of oxygen reduction product become severe. This study can help to determine which parameters are the most important for developing practical Li-air batteries. References 1. K. M. Abraham, Z. Jiang, J. Electrochem. Soc. 1996, 143, 1.2. H. G. Jung, J. Hassoun, J. B. Park, Y. K. Sun, B. Scrosati, Nature Chemistry 2012, 4, 579. 3.3 M. M. O. Thotiyl, S. A. Freunberger, Z. Peng, Y. Chen, Z. Liu, P. G. Bruce, Nature Materials 2013, 12, 1050.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-454**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Methanol Dehydrogenation at Au@Pt catalysts for Methanol oxidation

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

120th KCS General Meeting & Exhibition

Conference Date: October 18~20, 2017

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Code: **ELEC.P-455**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

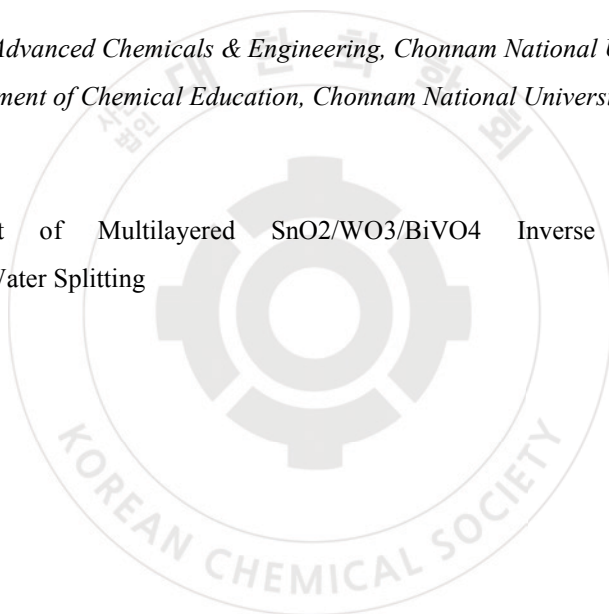
Cascading Alignment of Multilayered SnO₂/WO₃/BiVO₄ Inverse Opal Skeletons in Photoelectrochemical Water Splitting

Gun Yun, Soon Hyung Kang^{1,*}

Department of Advanced Chemicals & Engineering, Chonnam National University, Korea

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

Cascading Alignment of Multilayered SnO₂/WO₃/BiVO₄ Inverse Opal Skeletons in
Photoelectrochemical Water Splitting



Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-456**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The GOs supported Pt nanoparticles with high activity and stability for hydrazine electro-oxidation in a strong acidic solution

Jidang Kim, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

Pt nanoparticles have been particularly recognized as among the most promising catalysts for fuel cell applications because of their outstanding catalytic activity. However, the high prices and limited abundance of Pt resources hinder its commercial applications. Thus, Pt nanoparticles are generally used in a carbon-supported form (Pt/C catalyst) because of the cost reduction and increase in activity. However, the catalytic performances of Pt/C catalysts usually decline gradually due to their degradation under harsh operating conditions; the major reasons for Pt/C catalyst degradation are Pt dissolution and corrosion of the carbon support. Therefore, the development of Pt catalysts offering high activity, stability, and recyclability is currently a very popular research focus. In this study, we report a simple and effective process to prepare Pt nanoparticles-decorated GOs by using the amidation method on GOs surfaces. Amine groups were utilized as linkers to secure the Pt nanoparticles without agglomeration. The sample was characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The Pt nanoparticles decorated GOs exhibits higher activity in electrochemical reactions of hydrazine oxidation in a strong acidic solution than that of the reference systems. This synthetic approach should be broadly applicable for preparing GO-supported metal catalysts and markedly improves the catalytic activity.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-457**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Chitosan-based polymeric binder for highly-stable silicon anode in Lithium ion battery

Sang Ha Lee, Jeonghun Lee, Seon Kyu Yun, Mi suk Cho, Youngkwan Lee*

School of Chemical Engineering, Sungkyunkwan University, Korea

Here we demonstrate a novel binder material based on chitosan and rubber for silicon nanoparticle-based lithium ion battery anode. The chitosan and rubber was cross-linked, where various ratios between chitosan and natural rubber were adapted to optimize the mechanical and electrochemical properties. The mechanical and adhesive properties of cross-linked binder were investigated by using universal tensile machine, and its electrochemical properties were characterized by charge-discharge test and electrochemical impedance spectroscopy. It was found that the cross-linked chitosan-rubber with optimized composition can tolerate the stress generated by the volume variation of silicon particles, resulting in the outstanding cyclic stability. It might be due to tailored mechanical properties of binder material for silicon anode.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-458**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The High-Performance Silver Plasmonic Nano Structure Coupled with BiVO₄ Inverse Opal Photoelectrode to Improve the Water Oxidation

Maheswari balamurugan, Soon Hyung Kang^{1,*}

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

Developing a photocatalysis system to generate hydrogen from water is a topic of great interest for fundamental and practical importance. BiVO₄ Photocatalyst has suffered by the slow charge separation kinetics at solid/electrode interface that limits the photoelectrochemical performance (PEC). In order to minimize the poor properties, we modified the BiVO₄ IO photocatalyst with an effective silver Plasmonic Nano structure which was examined under light illumination. Silver Nano structure scatter propagating Plasmon's into photons in which light is coupled between BiVO₄ IO and silver metal. As a results the photonic crystal properties with the formation of a plasmonic band gap leads to a red shift in the electrode that allows harvesting and generating a larger portion of solar spectrum. The well-defined size, smooth surface and high crystallinity of silver Plasmon's facilitates fast electron transport to the photoelectrode.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-459**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemical detection of amyloid- β oligomers based on the signal application of nanostructured polypyrrole

JIELING QIN, Mi suk Cho, Youngkwan Lee^{*}

School of Chemical Engineering, Sungkyunkwan University, Korea

In this work, a novel impedance sensor was developed based on a transducer of carboxyl end-capped polypyrrole nanostructure electrode and a probe of cellular prion protein (PrPc) selectively cognitive of amyloid- β oligomer. The nanostructured PPy was electrochemically synthesized by one step template-free polymerization and then, the carboxyl group was introduced by the addition of pyrrole- α -carboxylic acid, which was covalently coupled with the amine group of PrPc. The morphology of the PPy was confirmed by scanning electron microscopy. The modification and the electrochemical properties of the electrode were characterized by cyclic voltammetry and electrochemical impedance spectroscopy. The modified sensor provided to be highly sensitive to amyloid- β oligomer in a broad detection range of 0.00001-0.1 nM. The high selectivity and sensitivity of the A β oligomer sensor can be used in practical for the early diagnosis of Alzheimer's disease.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-460**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Size and shape-dependent catalytic performance of gold nanostructures

Hyunjun An, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

Nanomaterials are used widely in a range of electrochemical applications, such as electrocatalysis, electrochemical analysis, and electrochemical synthesis, owing to their physical and chemical properties. Versatile synthetic routes to nanomaterials have been developed to allow control of the morphology, structure and surface chemistry, which are crucial parameters in both fundamental studies and applications. In the present study, a series of well-defined core-satellite Au nanoassemblies (CSNs) with different porosities, i.e. with the core-to-satellite gap distance controlled on a molecular scale, were synthesized. The effects of the interparticle distances on the ORR efficiency of the catalysts derived from the CSNs were investigated systematically by varying the length of the alkanedithiol molecular linkers ($\text{HS}(\text{CH}_2)_n\text{SH}$; $n = 4, 8, 10$). The series of as-prepared CSNs catalysts on carbon supports are denoted as CSNs(n)/C based on the length of the chain between the core and the satellites. This simple method is significant in preparing high-performance metal nanocatalysts with a well-controlled morphology, i.e. emphasizing the importance of tailored porosity in heterogeneous catalysis. Indeed, the electrocatalytic activity depends not only on the active site, but also on the surface morphology, particle sizes and surface area to volume ratio. The as-prepared CSNs exhibited unexpectedly high catalytic activity and a dominant four-electron pathway towards the ORR. This research was also supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-461**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile synthesis of carbon-supported porous manganese–iron nanocomposites as bifunctional electrocatalysts

Nhan Duy Pham, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

Efficient low-cost electrocatalysts are indispensable for electrochemical oxygen reduction reactions (ORR) and oxygen evolution reactions (OER). Typically, Pt-based nanoparticles are widely used as efficient catalysts to provide complete four-electron transport pathways with remarkably reduced overpotentials during ORR processes. However, the high cost and poor stability of Pt has led to the search for active non-precious metal/metal oxide catalysts that can replace Pt. On the other hand, OER plays a critical role in water splitting processes during solar fuel production or charge-discharge processes in rechargeable fuel cells and batteries. Unlike the ORR systems, transition metal oxides or perovskites are typically considered as excellent catalytic candidates for OER on account of their high activities and good stability. In this study, carbon-supported manganese-iron nanoparticles are successfully synthesized in various stoichiometries by using the reflux method followed by calcination at different temperatures for different times in the air. A combination of characterization techniques including transmission electron microscopy, scanning electron microscope, and the electrochemical analyzer was utilized to evaluate the structural, morphological and characterization of catalysts. This research was also supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-462**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Sulfur-doped graphene via electrochemical exfoliation of graphite and its electrochemical application

Jinheui Lee, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

Reduced graphene oxide has been shown to exhibit many interesting materials properties that are useful for electronic and electrochemical application, including nanoelectronics, electrocatalysis or sensors. However, the suitability of the material for these applications is limited by the fact that the graphene in its pure state exhibits zero band gap and that its electrochemical behavior resembles that of graphite. Doping of graphene with heteroatoms (such as hydrogen, nitrogen, and sulfur) can change the electron density in the graphene sheet and provide an electrode catalytic active site. Here, we have developed a simple chemical method to obtain bulk quantities of S-doped, reduced graphene oxide sheets (S-RGO) via electrochemical exfoliation of graphite in the presence of sodium thiosulphate acting as a sulfur source. The S-RGO materials are characterized by X-ray photoelectron spectroscopy, transmission electron microscopy, and Raman spectroscopy. We also investigate the electrocatalytic activity of the S-RGO catalyst for the oxygen reduction reaction (ORR) and compare it with RGO. This research was also supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-463**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemically synthesized all-carbon hybrid nanocomposites: Synthesis, characterization and their applications

Anh.T.N Nguyen, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

In recent years, carbon hybrid nanostructures have attracted attention because of their characteristics derived from both graphene and carbon nanoparticles (CNs). Combining the structure of graphene with CNs arise their unique properties, large surface area, and good water solubility, which make them are expected to be suitable for various application. Here, we report a facile and efficient approach to fabricate N-doped graphene decorated by CNs (NG-CNs) via electrochemical exfoliation of carbon precursor, such as graphite foils. Through direct nanoparticle nucleation in the presence of NG sheets, an NG-CN hybrid is developed as a highly efficient electrocatalyst for oxygen reduction reaction (ORR) in alkaline conditions. Electrochemical, transmission electron microscopy, and X-ray structure investigations revealed that the nucleation and growth method for forming all-carbon hybrids results in uniform dispersion of CNs on to the surface of NG. The all-carbon hybrids afforded much greater activity and durability than the physical mixture of NG and CNs. This research was also supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-464**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of Ru-Pd chain nanowires for bifunctional oxygen electrocatalysis in alkaline solution

Sunguk Noh, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

The development of active, robust, and bifunctional catalysts for both the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) is important and challenging. The key technology in the regenerative fuel cell, which consists of two separated subsystems: a fuel cell and a water electrolyzer, is the fabrication of bifunctional oxygen catalysts which promote both ORR and OER. Recently, it has been reported that the promising bifunctional oxygen catalysts are limited to several noble metals, such as Pt, Ir, Ru, IrO₂ and RuO₂. In the previous work, Ru and its oxides are unstable in the operating conditions although they display a high catalytic activity to OER. This presentation reports the facile synthesis and characterization of carbon-supported Ru-Pd chain nanowires (Ru-Pd/C). A series of Ru-Pd/C with various Ru/Pd weight percentage ratios were prepared by the spontaneous deposition of a Ru cluster on a Pd chain nanowires core using different Ru precursor concentration. The compositional/structural features were characterized by scanning electron microscopy equipped with an energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The electrocatalytic activity of the Ru-Pd/C for both ORR and OER in alkaline media was investigated by rotating disk electrode, and cyclic voltammetry. Indeed, the prepared Ru-Pd chain nanowires with a very low content of Ru exhibited significant electrocatalytic activity towards both ORR and OER. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-465**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Shape-dependent electrocatalytic behavior of Pd nanoparticles for the cathodic reduction of oxygen

Anh.T.N Nguyen, Nayun Jung, JUN HO SHIM*

Department of Chemistry, Daegu University, Korea

Precious metal nanocrystals play an important role in many industrial applications, such as catalysis, medicine, electronics, etc. In all of these applications, the size and shape of metal nanocrystals are critical parameters that must be controlled to maximize their value. In this study, we report an efficient synthesis of size and shape-controlled Pd nanostructure in an aqueous solution and their electrocatalytic activity for oxygen reduction reaction (ORR). The proposed synthesis was examined using L-ascorbic acid as a reducing agent of Pd²⁺ in the presence of both a stabilizer and a capping agent such as Pluronic F127. The resultant Pd nanoparticles have three different shapes, while their sizes can be controlled by using Pluronic F127 : KBr with different aspect ratios. Apart from this, a fine control of the nanoparticle shape can be achieved by the systematic variation of the experimental parameters. The structure, morphology and electrocatalytic activity of the Pd nanostructures is characterized by transmission electron microscopy (TEM) and electrochemical analyzer. This research was also supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2016R1D1A1B03930895).

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC.P-466

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Non-ideal behaviors of peroxyorganic acid to enhance oxidizing power

Jae Ku Jung, gyoyoon chae¹, hye ji kim¹, jeong dong kim¹, Won-Seok CHAE^{1,*}

Department of Research & Development, Scientific Agriculture Co.,Ltd., Korea

¹*Division of Life Science and Chemistry, Daejin University, Korea*

Hydrogen peroxide, which is widely used as an oxidizing agent for disinfection, could be increased in oxidizing power by synergy with organic acids. In this study, citric acid was used as an organic acid. The increased oxidizing power was confirmed by the potentiometry, and the cyclic voltammetry was used for confirming the reduction potential change and oxidation current disappearance of hydrogen peroxide. The non-ideal behavior of hydrogen peroxide titration with permanganate and of citric acid titration with hydroxide were observed. The disinfection power using the mixture was confirmed by a 5 minute contact disinfection test of harmful bacteria (*Escherichia coli* and *Staphylococcus aureus*), in which the concentrations of citric acid and hydrogen peroxide were

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Code: **ELEC.P-467**

Area: Electrochemistry

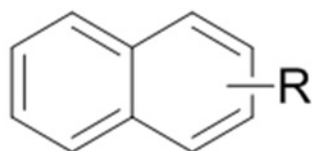
Type: Poster Presentation, Time: FRI 13:00~14:30

The Investigation of CV in Naphthalene Derivatives as High Energy Density Anolyte: Application for Redox Flow Battery

heung seop Lee, Chujin Ahn*

Department of Chemistry, Changwon National University, Korea

Redox flow battery (RFB) is a type of electrochemical energy storage devices. It is necessary to improve the energy density in RFB system. Herein we report the investigation on relationship between electrochemical properties of naphthalene derivatives. To do this we investigated the CV results depending on their different functional group



[R = H, Me, OMe, X, NO₂, etc.]

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-468**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Cobalt silicide nanowires based high-performance microsupercapacitors

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Separation and Conversion Materials Research, Korea Institute of Energy Research, Korea

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

The effectiveness of cobalt silicide nanowires grown on silicon substrate by chemical vapor deposition method as electrode material for micro-supercapacitors has been investigated. The as-synthesized cobalt silicide nanowires densely cover the silicon substrate and have small diameters of 40-70 nm. They showed the crystal structures and chemical composition of cobalt-rich silicides (Co₃Si, Co₂Si). Electrochemical measurements showed that the cobalt silicide nanowires exhibit high areal capacitance and good rate capability. The cobalt silicide nanowires grown on silicon substrates present many advantages for supercapacitor application, including high surface area, low resistivity, and good mechanical adhesion with the silicon substrate showing great promise for applications in micro-supercapacitors.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-469**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Surface functionalized porous carbon electrodes for enhanced electrochemical capacitor performance

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

Carbon-based electrochemical capacitors (ECs) are highly promising energy storage devices that can meet the demands of high power density and long cycle life but they exhibit a lower energy density compared to lithium ion batteries because of the electrostatic double-layer charge storage mechanism. To increase the energy density of ECs, hybrid electrodes which combine carbon and pseudocapacitive materials are being actively studied. Redox-active organic molecules are extremely attractive because they have large gravimetric energy density, low cost, mechanical flexibility, and chemical tunability.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-470**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

For improving electrocatalytic activity of refluxed graphene oxide(Re-G-O) Co(acac)₂ anchored on the Re-G-O for oxygen reduction reaction

Yunseok Shin, Sungjin Park^{*}

Department of Chemistry, Inha University, Korea

Organometallic complexes and carbon-based materials hybridization has been shown to enhance the catalytic performance in the oxygen reduction reaction (ORR). As chemical interactions between the metal centers and ligands are critical factors determining their tunable catalytic nature, it is important to understand the correlation between the chemical structure and catalytic performance of the hybrids. In this work, we synthesized the hybrids by the reaction of an organometallic complex Co(II)(acac)₂ (acac = acetylacetonate), with refluxed graphene oxide (Re-G-O) materials containing controlled amounts of oxygen atoms at room temperature. Experimental characterization of the hybrids reveals that Co(II)(acac)₂ is coordinated to oxygen containing groups in Re-G-O, generating organometallic species, Co-O₄-O. These hybrids showed better electrocatalytic activity for the ORR in alkaline media than Co-free Re-G-O materials. The results show that the Co-O₄ species is catalytically active for the ORR. We find that the best Co-O₄ catalyst for the ORR is produced by the use of reduced graphene oxide with a medium level of reduction.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

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Area: Electrochemistry

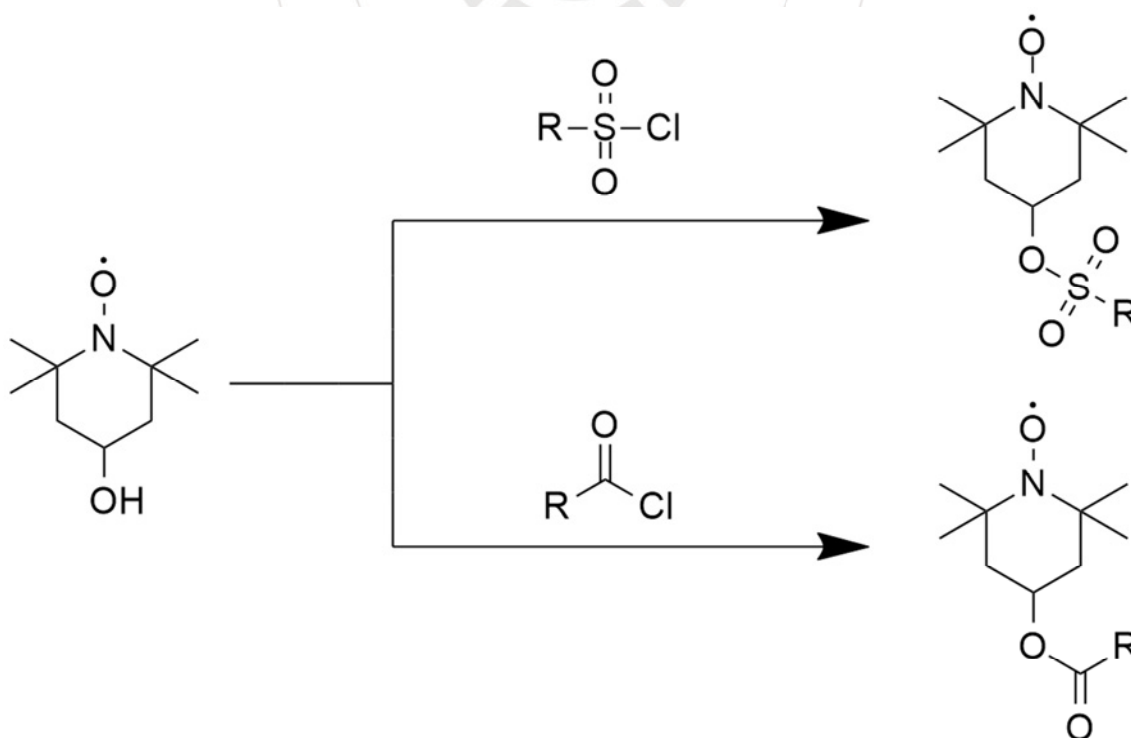
Type: Poster Presentation, Time: FRI 13:00~14:30

Preparation and Electrochemical Investigation of TEMPOL Derivatives : Apply to Redox Flow Battery

Hyunil Cho, Chujin Ahn *

Department of Chemistry, Changwon National University, Korea

Recently TEMPOL derivatives are interesting to organic catholyte in redox flow batteries(RFBs) for offering the possibility of wide potential windows. Here in we report the investigation on relationship between electrochemical properties of TEMPOL derivatives. To do this we prepared TEMPOL derivatives and investigated CV results depending on their different functional group.



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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-472**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Enhanced Electrochemical Stability of Electrolyte and Corrosion Suppression on GO Coated Current Collectors in Grignard Reagent-Based Electrolytes (APC) for Magnesium Ion Battery

Prabakar Richard, myoungho pyo*

Department of Printed Electronics Engineering, Suncheon National University, Korea

The electrochemical stabilities of some non-noble metal current collector electrodes in a magnesium ion battery (MIB) using Grignard reagent type electrolyte (APC) were investigated, wherein the chloride ions were responsible, which eventually lowered the corrosion resistance and electrolyte stability. In this investigation, we explore the possibilities of graphene oxide (GO) coatings on the non-noble metal current collector electrodes (Al, Cu and SS) via electrophoretic deposition. The GO-coated substrates displayed significantly large improvement in corrosion resistance, predominantly with a notable suppression of electrolyte decomposition at high potentials (4.0V), without the reversible deposition/stripping of Mg being affected. Studies showed a variance in the corrosion resistance which was dependent on the functional groups on graphene, coating effectiveness and thickness. We address that such a remarkable improvement by GO-coating is associated with electrostatic charge interaction between ion charges of electrolytes and surface-functional groups of GO. In addition, GO-coating does not aggravate the cathode performance of Mo_6S_8 , allowing the use of non-noble metals as current collectors as replacement to expensive Pt current collector electrode.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-473**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Real wastewater treatment for hydrogen production with microbial electrolysis cells

JunHyun Kim, Yongwon Jeon, Sunghyun KIM*

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Treating wastewaters from manufacturing processes is mandatory before discharging them to the environment. Domestic and industrial wastewaters often contain a certain level of organic substances which need biological treatment. Microbial electrolysis cells (MECs) are especially suitable for this purpose in that both wastewater treatment and hydrogen production can be achieved simultaneously. Microorganisms immobilized on the anode surface take organic substances as substrates, decomposing into carbon dioxide, protons, and electrons. Upon some external voltage bias, protons and electrons combine to hydrogen at the cathode under the anaerobic condition. Here we show that the exclusive H₂ production is possible when acetate was used as a substrate. Also, we have applied MEC technology to treat domestic wastewater for H₂ production. We found that CH₄ instead of H₂ was produced under the low voltage bias but H₂ portion increased with increasing bias. We present how the experimental conditions can change the gas composition and how to mainly produce hydrogen from wastewater.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-474**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Detection of Single Water/Oil Nanoemulsion Droplet using Electrochemical Collisions on an Ultramicroelectrode

Nhung Hoang, Thy Ho, Jun Hui Park^{1,*}, Byung-Kwon Kim^{*}

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

Herein, for the first time, research on water-in-oil (water/oil) emulsion droplets by electrochemical analysis has been reported. When the water/1,2-dichloroethane emulsion droplets collided with an ultramicroelectrode (UME), the blocking property of the droplets resulted in a “staircase” current decrease. Each “staircase” current decrease is associated with the collision of an emulsion droplet with the UME surface. The experimental collision frequency was proportional to the concentration of the emulsion droplet. In addition, the size of each water droplet was estimated from the magnitude of the “staircase” current decrease and the simulation data. Results obtained from the collision signals provide information about the size of each single droplet (nano- to micro-) and the pM level concentrations of the water droplets in the organic continuous phase.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-475**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Detection and Counting of Red Blood Cells by Electrochemical Collision Method

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Blood tests (e.g., red blood cell count) are very necessary for diagnosing and detecting blood diseases. Here, we have developed the electrochemical detection of red blood cells (RBCs) using single particle collision method. The staircase current decrease was caused by collision of RBCs on electrode, and providing quantitative information on the size as well as concentration of RBCs. As the result, the signals obtained by chronoamperometry (CA) measurement during a collision of RBCs with ultramicroelectrode (UME) showed high sensitivity in detecting anemia related diseases.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-476**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

The Electrochemical Measurement of Low Concentrations of Mercury in Aqueous Solution Using Emulsion Droplet Extractor

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Mercury is one of the most hazardous heavy metals to human health and is hard to remove from the environmental system due to its extended half-life time and lack of decomposition. Thus, it is highly required to analyze the quantitative description of mercury in aqueous solutions through a simple, fast, and sensitive technique. In the present study, amperometric technique based on the emulsion droplet reactor (EDR) method was performed to observe the electrochemical detection of mercury ions in low concentrations. Here, the emulsion droplets were used as an extractor and reactor for mercury ions. As a result, we could measure stochastic collision events as current spikes at a cathodic potential after the contact between the emulsion droplets and electrode. In comparison with other methods, this technique permits rapid and sensitive analysis without further modification of electrode surface.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-477**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Domestic wastewater treatment with a photo-assisted microbial electrolysis cell

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Department of Bioscience and Biotechnology, Konkuk University, Korea

Microbial electrolysis cells (MECs) are a promising technology for wastewater treatment and the simultaneous production of energy gases such as hydrogen and methane. In most MEC studies, synthetic wastewater which contains pure compounds (acetate or glucose) as a substrate have been examined for effective hydrogen production. External voltage bias of 0.114 V or more must be applied to operate MECs due to the thermodynamic barrier for hydrogen production. To resolve this problem, we have developed a photo-assisted microbial electrolysis cell (PAMEC) for domestic wastewater treatment which consists of a bioanode and a p-type semiconductor photocathode. With an aid of solar energy, our PAMEC system continuously produced methane with 55 A/m³ current density with simultaneous COD removal of 66 % at 0.8 V of external applied voltage under visible light illumination. These results show the possibility of a PAMEC as a future energy source that produce hydrogen and methane from wastewaters.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-478**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Magnesium aluminate triflate complex (MATC) as a new electrolyte system with wide electrochemical window for magnesium ion batteries

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Magnesium (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)]. There are two major issues in developing the Mg rechargeable batteries, which are: (i) relatively narrow potential windows of Mg^{2+} -based electrolytes; (ii) slow diffusion of Mg^{2+} ions in active materials. The first successful Mg deposition/dissolution in Mg^{2+} electrolytes was reported by Aurbach group, using Mg organohaloaluminate salts (APC). Inspired by this seminal work, researchers tried to increase the potential window (up to 2.3 V vs. Mg in APC-type) and to replace the toxic Grignard-based electrolytes. Various non-Grignard type electrolytes such as $\text{MgCl}_2\text{-AlCl}_3$ (MACC), $\text{Mg}(\text{HMDS})_2\text{-AlCl}_3$ and $\text{MgCl}_2\text{-Mg}(\text{TFSI})_2$ have been reported. However, these electrolyte systems show relatively lower anodic limit, poor coulombic efficiency and/or battery performance. Herein, we report the combinations of magnesium triflate (MgTf_2) and Lewis acid AlCl_3 in ether type solvent (Diglyme) which displayed reversible Mg plating/stripping, high anodic limits, and good reversible Mg^{2+} insertion/de-insertion for the Mo_6S_8 cathode. The system we evaluated can be represented as $x\text{M MgTf}_2 + y\text{M AlCl}_3/\text{Diglyme}$ and the active species [$\text{Mg}_2\text{Cl}^{3+}$] was identified and confirmed by ESI-mass spectroscopy. Electrochemical stability of electrolyte and cyclic stability of Mo_6S_8 in this electrolyte were studied.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-479**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Enhanced Electrocatalytic Reduction of CO₂ to CO via Gold-Based Clusters

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¹*Department of Chemistry, Yonsei University, Korea*

As energy and environmental problem is being serious, electrochemical CO₂ reduction reaction (CO₂ RR) to value-added products is regarded as a useful method and becomes gradually notable in these days. Among the products to which CO₂ can be reduced, CO has advantage to form a practical syngas with H₂. However, efficient system for CO₂ reduction to CO selectively has not been realized until now, because there are some problems such as complexity of CO₂ RR and competition with hydrogen evolution reaction (HER). Herein, we use Au₂₅(SC₆H₁₃)₁₈ and Au₃₈(SC₆H₁₃)₂₄ nanoclusters as electrocatalysts with high selectivity for CO. The clusters are mixed with carbon black and nafion, and casted on gas diffusion layer. Constant potential electrolysis was then carried out for 1 hour, in aqueous solution containing KHCO₃ and KCl. For Au₂₅ cluster, the current density reaches up to 32mA/cm² at -1.06V vs. RHE. For Au₃₈ cluster, the current was found to be 42mA/cm² at same potential, about 1.3 times higher than that of Au₂₅, with maximum CO Selectivity of 97% at -0.86V. Moreover, electrolyte conditions that play an important role in CO₂ reduction, higher current density and selectivity for CO were examined. Systematic investigations of the electrolyte compositions reveal that the bicarbonate concentration in the electrolyte profoundly affects the local and bulk pH, which control the catalytic activity and selectivity.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-480**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Temperature Dependent Crystal Structure of MoO₃ for Lithium-Ion Batteries

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Department of Chemistry, Sungkyunkwan University, Korea

Secondary battery systems are considered as an essential energy storage system (ESS). Among them, lithium-ion batteries (LIBs) have attracted considerable attentions because they could be applied as the power source for small portable devices as well as ESS for very large grid systems. As a cathode material for LIBs, molybdenum-based materials were used because they have advantages such as low cost, abundant resources and non-toxicity. Also, it can be applied at Sodium-ion battery (SIB) area. In this work, nanobelt and hexagonal prism structured MoO₃ were synthesized by hydrothermal method. The crystal structure were dominantly dependent on the temperature during the synthetic procedure. When the synthetic temperature was controlled at 120 oC, hexagonal MoO₃ was synthesized. But 140 oC and 160 oC allowed hexagonal MoO₃ and orthorhombic MoO₃ were formed at the same time. When the hydrothermal temperature was raised to 200 oC, only orthorhombic MoO₃ was synthesized. Temperature dependent redox capacity of MoO₃ was also presented. Nanobelt and hexagonal prism structures were characterized by Scanning electron microscope (SEM), X-ray Diffraction (XRD), Energy dispersive X-ray spectroscopy (EDS). Electrochemical properties were measured by Cyclic Voltammetry (CV).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-481**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Estimation of Catalytic Activity of Gold Nanoparticles toward CO₂ Reduction Using Scanning Electrochemical Microscopy

YEOMIN KIM, ara jo, Youngmi Lee^{*}, Chongmok Lee^{*}

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

Recently, CO₂ reduction has attracted great attention in the field of renewable energy because the products of CO₂ reduction, such as CO, CH₄, HCOO⁻ and C₂H₄, are useful for recyclable energy sources. In fact, the selectivity of the product is an important challenge for using it as an energy source in a practical manner. Unlike other metals, it is generally known that Au has good selectivity for CO₂ reduction products. The electrochemical reduction products of CO₂ at Au are known as mostly CO and H₂. The selectivity of CO among CO₂ reduction products could be close to 100% if CO₂ reduction occurs at more positive potential than that of H₂ generation. In this study, we synthesized AuNPs/CB which is nano-sized gold particles (AuNPs) on carbon black (CB). The results of the electrochemical study show that our catalyst is effective not only in oxygen reduction but also CO₂ reduction. In particular, we have analyzed the electrochemical activity of AuNPs/CB toward CO₂ reduction using scanning electrochemical microscopy (SECM). SECM is an electrochemical scanning probe technique where the tip current caused by an electrochemical reaction is measured. If the tip electrode moves to the substrate electrode very closely, it can re-oxidize the reduction product from substrate by control of electrode potentials via a bipotentiostat. The substrate electrode is glassy carbon electrode loaded with AuNPs/CB and the tip electrode is the electrochemical CO-sensor. Using this technique, we have tried to analyze the exact onset potential of the CO₂ reduction in electrocatalytic system.

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Code: **ELEC.P-482**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrocatalytic Oxygen Evolution Reaction on Electrospun Iridium-Cobalt Mixed Oxide Nanotubes

AREUM YU, Chongmok Lee, Myung Hwa Kim¹, Youngmi Lee^{*}

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

Mixed oxide nanocomposites consisted of both Ir and Co ($\text{Ir}_x\text{Co}_{1-x}\text{O}_y$, $0 \leq x \leq 1$) via electrospinning and calcination are prepared as high performance electrocatalysts for oxygen evolution reaction (OER). The efficiency of water splitting is limited by the significant overpotential of the OER, because OER which is kinetically slow anodic half reaction of water. The morphologies and compositions of the synthesized $\text{Ir}_x\text{Co}_{1-x}\text{O}_y$ nanotubes are investigated with field-emission scanning electron microscopy (FE-SEM), energy dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). X-ray diffraction (XRD) and Raman spectroscopy show the change of the structure occurred with blending of two elements. Electrochemical activities of diverse $\text{Ir}_x\text{Co}_{1-x}\text{O}_y$ nanotubes for OER are characterized with rotating disk electrode voltammetry in 1 M NaOH aqueous solution. Among various compositions of $\text{Ir}_x\text{Co}_{1-x}\text{O}_y$, $\text{Ir}_{0.46}\text{Co}_{0.54}\text{O}_y$ nanotubes are examined to have the highest OER activity (the least positive onset potential, greatest current density and low Tafel slope) which is higher than commercial Ir/C. In addition, the $\text{Ir}_{0.46}\text{Co}_{0.54}\text{O}_y$ nanotubes also possess a high stability during repetitive OER scans in alkaline electrolyte. 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).

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-483**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Sonochemical Synthesis of ZnO-ZnS Composite for Enhanced Photoelectrochemical Water Oxidation

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The ultrasonic-assisted synthesis method provides a fast, simple, and large scale route for synthesizing desired materials under ambient conditions. Here, the facile preparation of ZnO-ZnS composite on a fluorine-doped tin oxide (FTO) substrate. The composite was synthesized by sequential nanoscale reactions involving the preparation of ZnO and conversion of the ZnO surface into a ZnS shell on the FTO substrate, using an in situ sonochemical method. The ZnO-ZnS composite showed improved photocurrents compared to ZnO for the water oxidation reaction. During the water oxidation reaction, the ZnS shell passivates the surface-defects of the ZnO, which results in enhanced charge separation in the ZnO nanorods and higher performance.

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Code: **ELEC.P-484**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

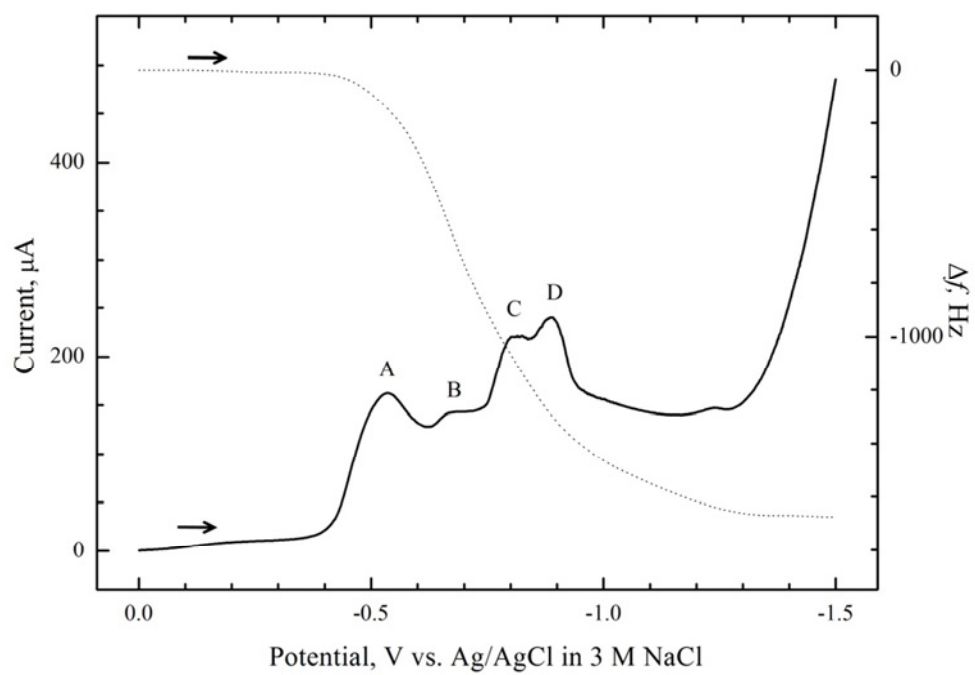
Electrodeposition of Cobalt Selenide Thin Films: A Combined Voltammetry/Electrochemical Quartz Crystal Microgravimetry Study

Hyung-woo Jee, YunHyeok Jang¹, KONGSHIK RHO¹, Ki Jung paeng, Noseung Myung^{1,*}

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The mechanism of electrodeposition of cobalt selenide (CoSe) thin films was investigated by the combined application of linear sweep voltammetry (LSV) and electrochemical quartz crystal microgravimetry (EQCM) on Pt-coated quartz electrodes. Cobalt selenide films were electrodeposited on the Pt surface from 0.1 M Na₂SO₄ electrolyte solution containing 5 mM SeO₂ and 5 mM Co(CH₃COO)₂ by linear sweep voltammetry. Four cathodic waves were observed during the linear scans and the reactions corresponding to these waves were investigated with LSV and EQCM. Combined stripping voltammetry and EQCM showed that CoSe was electrodeposited via two routes: (1) Underpotential deposition of Se followed by deposition of cobalt as CoSe; and (2) Reaction of Co(II) with electrogenerated Se(-II) to result in CoSe. Compositional analyses revealed that the electrodeposited films contained CoSe and free Se, depending on the deposition potential. However, no cobalt was found in the films due to chemical (galvanic) instability of the cobalt film in the deposition bath.



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Code: **ELEC.P-485**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Facile Synthesis of Bi₂S₃ Nanostructure for Enhanced Photoelectrochemical Water Oxidation

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Department of Chemistry, Mokpo National University, Korea

The ultrasonic-assisted synthesis method provides a fast, simple, and large scale route for synthesizing desired materials under ambient conditions. The Bi₂S₃ nanostructure was synthesized by direct growth on the FTO substrate, using an in situ sonochemical method. Photoelectrochemical water splitting is a light-driven chemical process over the surface of a semiconductor that can produce hydrogen from water. The prepared Bi₂S₃ nanostructure showed improved photocurrents compared to various Bi₂S₃ films for the sulfite oxidation and water oxidation reaction.

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Code: **ELEC.P-486**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Sensitive chemiresistive H₂O₂ gas detection on the ppb level based on graphene decorated with Ag nanowires

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In this study, we demonstrate single-layer graphene decorated with Ag nanowires (AgNWs) for sensitive and selective H₂O₂ gas sensing. The AgNWs were synthesized by typical polyol method. Single-layered graphene was grown using chemical vapor deposition (CVD) technique and doping with AgNWs was achieved using simple spin-coating pathway. The developed composite have been intensively studied using various characterization methods (SEM, EDS, XPS, and XRD). Our study revealed uniform distribution of AgNWs throughout the graphene substrate. The average diameter of AgNWs is 45 nanometers, with (111), (200) and (220) crystallographic planes. The doping changed the electronic properties of graphene, achieving a drastic resistivity change in the presence of H₂O₂ gas by converting metallic silver (Ag) to silver oxide (Ag₂O), which is a p-type semiconductor. This conversion changes the concentration of charge carriers in the conduction channel of graphene and thus allows to provide real-time H₂O₂ level monitoring at ambient temperature with a fast response and recovery under UV radiation. Doped graphene has demonstrated the ability to simultaneously, selectively and repeatedly sense H₂O₂ gas with the saturation time of around 4 min, and with the limit of detection being below 500 ppb.

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Code: **ELEC.P-487**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Fabrication of enhanced Screen Printed Carbon Electrodes (SPCEs) modified by nanomaterial, and its preparation method

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The Screen-Printed Carbon Electrodes (SPCEs) have found wide use as sensing platforms due to their simple fabrication, customizability in terms of geometry and composition, and relatively low cost of production. SPCEs mixed nanomaterials have beneficial electrochemical properties that are enhanced electron transfer rate at a lower potential and catalyzed electrochemical oxidation. To optimize condition, SPCEs mixed nanomaterials are used mainly Electroanalytical methods. Electroanalytical methods are more advantageous such as simple, low-cost, portable, easy-to-use and miniaturizing. These methods also consume less power and don't require transparent samples and directly convert the underlying chemical reaction into readable electronic digital signal. Lastly, The SPCEs mixed nanomaterials characterized by SEM, EDS, FT-IR and EIS. The enhanced SPCEs can be applied to biosensing system of heal care and point of care.

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Code: **ELEC.P-488**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

High Electrocatalytic Performance of Molecularly coordinated Co-based Active species on Carbon nanotubes for the Oxygen reduction reaction

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Hybrid systems in which molecule-cobalt based active species are combined with nanoscale materials may offer valuable routes to enhance catalytic performances for electrocatalytic reactions. The development of rationally designed, cost-effective, efficient catalysts for the oxygen reduction reaction (ORR) is a crucial challenge for applications in fuel cells and metal-air batteries for energy storage. A new hybrid ORR catalyst has been synthesized through a well-defined reaction between Co-based organometallic molecules and N-doped multiwalled carbon nanotubes (MWCNTs) at room temperature. The hybrid ORR catalyst shows excellent catalytic performance with an onset potential of 0.95 V [vs. the reversible hydrogen electrode (RHE)], superior durability, and good methanol tolerance in alkaline electrolytes. Chemical and structural characterization after many reaction cycles reveals that the Co-based organometallic species maintained the original structure of cobalt(II) acetylacetonate with coordination to the heteroatoms of the MWCNTs. A thorough electrochemical investigation indicates that the major catalytically active site is Co-O4-NCNT.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-489**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis of NiO-Embedded Carbon Sheet Using Salts and Polymer Reactions as an Anode Material for Lithium-Ion Batteries

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Serious environmental pollution and rapid depletion of fossil fuel reserves have facilitated the development of alternative energy conversion/storage systems in the past few decades. Lithium-ion batteries (LIBs) have recently been the most attractive means to store electric energy because of the low environmental impact, high energy density, and long cycle life. Nevertheless, the conventional LIBs using graphite as an anode have limitations to meet the increasing demands for high performance batteries due to its low theoretical capacity (about 372 mAh g⁻¹) and the lithium dendrites formation on graphite surface. NiO has been considered as an alternative anode material with its high theoretical capacity (about 718 mAh g⁻¹), nontoxicity, and low cost. However, NiO suffers from severe volume changes, rapid fading due to particle aggregations, and poor electronic conductivity during long-term cycles. As an effort to solve these issues, NiO-embedded carbon sheets (NiOC) were synthesized in this work. The carbon sheets were synthesized by polymerization reactions of citric acid and ethylene glycol with salts (NaCl and KCl) as structural templates. The NiOC composite exhibited the significantly improved cycling performance than bare NiO at 0.1 C rate in the 0.0-3.0 V voltage range.

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Code: **ELEC.P-490**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Enhanced Electrochemical Performances of the Li_3VO_4 with Surface Nitrogen-Doped Carbon Coating Thin Layers for Lithium-Ion Batteries

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Lithium vanadate (Li_3VO_4) has been recently reported as a promising anode material for lithium-ion batteries (LIBs) because of its relative high capacity (394 mAh g^{-1}) than graphite (372 mAh g^{-1}), small volume changes, and low cost. However, Li_3VO_4 (LVO) suffer from poor rate capabilities owing to its low electrical conductivity. In this study, nitrogen-doped carbon coated Li_3VO_4 (NC-LVO) was synthesized with dopamine (DA) as carbon source by a facile hydrothermal method and subsequent thermal treatments. Remarkably, the thickness of nitrogen-doped carbon coating layers could be controlled by simply adjusting the coating time using polydopamine (PDA). The NC-LVO sample exhibited the enhanced reversible capacity of about 426 mAh g^{-1} during 100 cycles at 0.5 C rate ($1 \text{ C} = 394 \text{ mA g}^{-1}$) in the voltage ranges of 0.01-3.0 V. Moreover, the NC-LVO also showed the improved rate capabilities at various current densities (0.1-20 C). The diffusion constants of the pristine LVO and NC-LVO electrodes were also analyzed by cyclic voltammetry (CV) measurements.

Conference Date: October 18~20, 2017

Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-491**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Determination of chromium(VI) using a gold-conducting polymer composite electrode

Min Ouk Park, Won-Chul Lee, Yoon Bo Shim*

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The dealloyed-AuNi-conducting polymer composite prepared by the potential step method is demonstrated for the detection of Cr(VI). The nanostructured electrode surface shows well-defined a voltammetric peak for the reduction of Cr(VI) at ~0.5 V. The modified electrode was characterized employing electrochemical and surface analysis methods. Experimental variables affecting the analytical performance were optimized. Interference effects of foreign metal ions having similar redox potentials were also investigated. The dynamic ranges of linear sweep voltammetry (LSV) and square wave voltammetry (SWV) for the target ion were between 1.0 ppb and 10.0 ppm, respectively with the detection limits of 0.85 ± 0.25 ppb ($n=3$) and 0.25 ± 0.05 ppb ($n = 3$). The reliability of the method for point-of-analysis was evaluated by analysing a standard reference material and water samples.

Conference Date: October 18~20, 2017

Venue: Kimdajeung Convention Center, Gwangju

Code: **ELEC.P-492**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Glucose sensor based on enzyme bonded- conducting polymer formed on metal alloy in hierarchical structure

Won-Chul Lee, Kyeongdeok Seo, Yoon Bo Shim *

Department of Chemistry, Pusan National University, Korea

A novel amperometric sensor for glucose was developed by enzyme bonded-conducting polymer coated on the hierarchically structured metal alloy (Au, Zn, Ni, Cu, Co, etc.). Poly-3'-(carboxylic acid)-2,2':5',2''-terthiophene (pTTCA) and poly-3'-(benzoic acid)-2,2':5',2''-terthiophene (pTTBA) were examined as the probe material. The sensor probe was prepared by electrochemical formation of enzyme-conducting polymer layer on a metal alloy using normal pulse voltammetry (NPV) and chronoamperometry (CA). The characterization of each layer was performed using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy (EDS). Experimental parameters were optimized in terms of pH, temperature, applied potential, deposition potential and deposition time. The proposed sensor exhibited highly stable and short response time (< 1s). The linear dynamic range was between 30 μ M and 5 mM with the detection limit of $5.3 \pm 0.42 \mu$ M.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-493**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Synthesis, electrochemical, and spectroelectrochemical properties of poly(3-([2,2':5',2''-terthiophen]-3'-yl)-5-aminobenzoic acid)

Kyeongdeok Seo, Won-Chul Lee, Yoon Bo Shim *

Department of Chemistry, Pusan National University, Korea

The functionalized conductive polymer of the terthiophene derivative, 3-([2,2':5',2''-terthiophen]-3'-yl)-5-aminobenzoic acid (TTABA) was firstly synthesized and monomer structure was confirmed with ¹H NMR and mass spectroscopy. The maximum UV-visible absorption and PL emission bands of TTABA monomer were observed at 346nm and 488 nm, respectively. Poly TTABA was characterized by in-situ UV-Vis spectroscopy, AFM, FE-SEM techniques. Spectroelectrochemical experiments were performed to observe the absorption bands of the pTTABA film in the neutral and oxidized forms. The DCVA analysis of pTTABA shows the absorption bands at 470, 759 and 948 nm corresponding to the π - π^* transition, polaron, and bipolaron formations, respectively. The polyTTABA film shows reversible multiple color transition within 0.6 s (from brownish-yellow (at 0.0 V) to blue (at +1.3 V)) when the potential switches between the reduced and oxidized states.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-494**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemical Zinc Ion Intercalation and Structural Properties of Chevrel Phase and Rhombohedral Zinc Hexacyanoferrate for Post Li-Ion battery

Munseok Chae, Seung-Tae Hong*

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

Zinc ion batteries have received attention as one type of these multivalent ion batteries (post-LIBs) due to their potential applications to large-scale energy storage systems. Zinc has various merits, including safety, abundance, low cost, environmental friendliness, and large theoretical capacity of 820 mAh/g. Rhombohedral zinc hexacyanoferrate [$\text{Zn}_3\text{Fe}_2(\text{CN})_{12}$ or ZnHCF] has also been shown to intercalate Zn^{2+} ions into large, open sites of the porous three-dimensional (3D) framework in an aqueous electrolyte. There was significant structural change during the electrochemical zinc insertion. However, the crystal structure of the zinc-inserted phase has not been determined yet. One of the Chevrel phases, $\text{Zn}_x\text{Mo}_6\text{S}_8$ phase ($0 \leq x \leq 2$), has been noticed as a potential electrode material for zinc ion batteries. $\text{Zn}_2\text{Mo}_6\text{S}_8$ was prepared from Mo_6S_8 electrochemically in aqueous as well as organic Zn-containing electrolytes, with two potential plateau regions, one for $0 \leq x \leq 1$, and the other for $1 \leq x \leq 2$. It has been noted that $\text{Zn}_2\text{Mo}_6\text{S}_8$ seems to be obtained only via the topotactic insertion reaction but not by direct synthesis at high temperatures, and its crystal structure has not yet been determined. In this study, we present the electrochemical insertion and extraction properties of Zn^{2+} in $\text{Zn}_x\text{Mo}_6\text{S}_8$ ($0 \leq x \leq 2$) and $\text{Zn}_{3+x}\text{Fe}_2(\text{CN})_{12}$ ($0 \leq x \leq 0.75$) in aqueous or organic electrolytes, and finally the crystallographic analyses of the electrochemically obtained phases, where the new structures of $\text{Zn}_2\text{Mo}_6\text{S}_8$ and $\text{Zn}_{3.75}\text{Fe}_2(\text{CN})_{12}$ were determined for the first time. In order to locate the inserted zinc positions, the technique of structural determination from powder diffraction data was applied.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-495**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Separation analysis of neurotransmitters using a AC field applied- microfluidic channel with an amperometric sensor

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A separation analysis of various neurotransmitters in human urine and blood samples was performed using AC field applied microfluidic channel device, attached with an external amperometric sensor. The sensor was fabricated by electropolymerization of poly (2,2':5',5"-terthiophene-3'-p-benzoic acid) (pTBA) and porous carbon (PC) layer onto the screen printed electrode (SPCE), followed by covalent immobilization of a redox active mediator. The sensor probe material was characterized employing electrochemical impedance spectroscopy (EIS), X-ray photoelectron spectroscopy (XPS) and various other electrochemical methods. The experimental parameters affecting the analytical performances for dopamine, norepinephrine, epinephrine, serotonin, 3, 4-dihydroxy-l-phenylalanine, 5-hydroxyindoleacetic acid, and 5-hydroxytryptophan are optimized. The reliability of the analytical method was demonstrated by determining seven neurotransmitters (DA, NE, EP, 5-HT, L-dopa, 5-HIAA and 5-HTP) in human urine and blood samples.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-496**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electropolymerization of thiophene-based monomers and electrochemical properties of synthesized conducting polymers

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Conducting polymers are currently attracting significant interest worldwide because of their potential applications in energy storage devices, electrochromic devices, and light emitting diodes. Electrochemical synthesis of conducting polymers offers several advantages; rapidity, simplicity, generation of the polymer in the doped state and easy control of the amount (film thickness) generated. In this study, cyclic voltammetry, electrochemical impedance spectroscopy, EQCM (electrochemical quartz crystal microbalance) and ultraviolet-visible spectroelectrochemistry have been performed to look at the processes of electropolymerization of the thiophene-based compounds and their electrochemical behavior. Cyclic voltammetry is used to characterize and polymerize the monomers. Electrochemical impedance spectroscopy shows surface property of the polymer-coated electrode. EQCM exhibits the amount of polymer attached to the electrode surface. Ultraviolet-visible spectroelectrochemistry is used to know how the optical properties of the conducting polymers and the monomer change.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ELEC.P-497

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Continuous glucose monitoring sensors modified by nitric oxide-releasing nanofiber for improving biocompatibility: Lifetime in freely-moving rat model with a wireless system

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Continuous glucose monitoring provides maximal information about shifting blood glucose levels throughout the day and facilitates the decision-making for optimal treatment of the diabetic patients. Designing in vivo glucose biosensor for clinical use, however, remains a significant challenge due to poor biocompatibility. Indeed, surface fouling affects the long-term utility of such devices by reducing glucose diffusion to the sensor and increasing the risk of infection. To remove or reduce such surface biofouling, a number of strategies have been explored including modifying the outer surfaces of biosensors with a range of polymeric membranes that resist protein adhesion. Unfortunately, these strategies have not dramatically improved the long-term performance of in vivo sensors. With the discovery of nitric oxide (NO) as a potent antithrombotic agent, the study of NO has been extended to the field of biomaterials. Due to its short half-life (i.e.,

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-498**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

A Chemically Modified Electrode with Polyaniline Derivatives: Experimental and Theoretical Mechanism Studies

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Carbon monoxide (CO) which is naturally produced by the action of heme oxygenase in the human body, plays diverse physiological roles as a signaling molecule. Abnormalities in its metabolism have been linked to a variety of diseases, including hypertension, neurodegeneration, heart failure, and inflammation. Therefore, the reliable detection of CO in vivo is essential to elucidate its numerous biological functions. However, the electrochemical measurement of CO has been challenging due to its low concentration, rapid diffusion, and severe interference from other electrochemically active species (e.g., nitric oxide, nitrite, ascorbic acid, and uric acid). Indeed, the utility of a tin (Sn)-deposited Pt electrode (previously known as an amperometric CO sensor) has been hindered by significant interference from nitric oxide (NO). The elimination of NO interference in the CO sensor development is one of the important factors, because CO's biological functions are closely related to NO's ones. Herein we report on a novel amperometric CO sensor with superior sensitivity and selectivity (especially over NO) via use of aniline derivatives as a sensing membrane. The films of aniline or its derivatives are deposited on a Pt electrode by electropolymerization (i.e., cyclic voltammetry). The sensing mechanism and the effect of electropolymerization conditions (e.g., scan rate, number of scan cycles, and types of anions doped during polymerization) will be discussed. The effect of dopant anions (e.g., hydrogen sulfate, dodecyl sulfate, and tetraborate) on sensor performance will be also evaluated. Furthermore, to investigate the substituent effect of aniline derivatives on sensor performance at the atomic level, the density functional theory (DFT) studies have been carried out with a series of aniline derivatives ortho-substituted with electron donating (e.g., methyl and ethyl) or electron withdrawing (e.g., fluoro, chloro, bromo, carboxylic, trifluoromethyl, and sulfonic) groups. The calculations are performed at unrestricted UB3LYP/6-31G(d) using the Gaussian 09 package with the dimer model of aniline derivatives.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **ELEC.P-499**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

Electrochemical immunosensors using fragmented antibody (Fab') and electrochemically active nanoparticles for diagnosis of allergic rhinitis

Sanggyeong Shin, Kihak Gwon, Jae Ho Shin*

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Electrochemical immunosensors based on antibody provide a rapid and convenient approach for sensitive and specific diagnosis. Despite many advantages, it is still a challenge to find new approaches that could improve the simplicity, specificity, and sensitivity for clinical uses. To enhance performance of antibody based immunosensors, it is particularly important to develop label-free detection methods. Several strategies to achieve label-free immunoassays have been demonstrated by using fluorescence, electrochemistry, quartz crystal microbalance (QCM), and surface plasmon resonance (SPR) spectroscopy. Herein we reported on a novel approach to design a label-free immunosensors via use of electrochemically active nanoprobe such as ferrocene (Fc)-modified silica nanoparticles. The fragmented antibody (i.e., Fab'; regular molecular weight of 50 kDa) immobilized on a gold electrode leads to changes in the interfacial electron transfer properties. The surface coverage with target proteins specifically bound to Fab' prohibits the access of electroactive probes to the electrode surface. To amplify such blocking effects associated with target protein-Fab' complex formation, Fc-modified silica nanoparticles are utilized as a scaffold to design macromolecular electroactive probes. Various conjugation techniques and addressed fabrication methods for Fab' oriented immobilization on a gold surface will be evaluated. Furthermore, we investigate the feasibility of applying the novel concept to develop the label-free, Fab'-based immunosensor to detect the biomarkers in allergic rhinitis such as Clara cell protein 16, tryptase, eosinophil cationic protein, and albumin. Finally, four biomarkers in artificial nasal discharge are simultaneously determined with multi-array sensor system equipped in a microfluidic device.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ELEC.P-500**

Area: Electrochemistry

Type: Poster Presentation, Time: FRI 13:00~14:30

One-step electrochemical co-reduction synthesis of electrochemically reduced graphene oxide (ERGO) and gold nanoparticles (AuNPs) nano hybrid composite for electrocatalytic detection of dopamine

Chang-Seuk Lee, sujean Shim, Tae Hyun Kim*

Department of Chemistry, Soonchunhyang University, Korea

Here, we fabricated the electrochemically reduced graphene oxide (ERGO) and gold nanoparticles (AuNPs) nano hybrid composite that was utilized successfully for the electrocatalytic detection of dopamine (DA), ascorbic acid (AA), and uric acid (UA), simultaneously. ERGO/AuNP nano hybrid composite was modified on glassy carbon electrode (GC) by graphene oxide (GO) using cyclic voltammetry (CV) technique. The ERGO/AuNP/GC electrode was obtained using graphene oxide (GO) and aurate ion (Au^{3+}) mixed solution (0.3 mg mL^{-1} GO, 0.3 mg mL^{-1} Au^{3+} in 10 mM PBS buffer solution) by scan from -1.5 V to 0.8 V (vs. Ag/AgCl reference electrode) three times at a scan rate of 10 mV s^{-1} . The ERGO/AuNP/GC was characterized by scanning electron microscopy (SEM), Raman spectroscopy, contact angle measurements, electrochemical impedance spectroscopy, and cyclic voltammetry (CV). The electrochemical performance of the ERGO/AuNP/GC with respect to the detection of DA, AA and UA in 0.1 M PBS (pH 7.4) was investigated by differential pulse voltammetry (DPV) and amperometry. The ERGO/GC exhibited three well-separated voltammetric peaks along with the increased oxidation currents in DPV measurements, which enables simultaneous and individual detection of DA, AA and UA. Detection limits were found to be $0.8 \text{ }\mu\text{M}$, $30 \text{ }\mu\text{M}$ and $10 \text{ }\mu\text{M}$ for DA, AA and UA, respectively, with S/N ratio of 3 using the amperometric $i-t$ curve technique.

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Code: **EDU.P-501**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Suggestion of Explaining Method as Process Viewpoint in Conjunction with Buoyancy and Density

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The phenomenon of floating and sinking is very common in our surroundings, so is dealt from childhood. But not only students but teachers are at an alternative conception level. In chemistry class, this phenomenon is explained using density. The explanation using density has the advantage that the determination of the outcome of this phenomenon is simple, but there is a lack of understanding as to why this density explains this phenomenon. The phenomenon of float or sinking cannot be explained by the material itself, and the fluid and the object must be considered at the same time. In addition, this phenomenon has a series of processes that float or sink. To include these two things, the approach of explaining this phenomenon should be process viewpoint. We used the lever as a visible tool for this suggestion. This explanatory approach helps to recognize the cause of this phenomenon as gravity, and has an educational value that makes it possible to understand that this phenomenon is caused by the relationship between materials, not the properties of the material. This can provide an understanding of why explanation using the density can explain this phenomenon. In addition, because we use the basic science concept of volume and mass, students can learn this phenomenon's principle scientifically before learning the density as upper science concept.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU.P-502**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Development of a program to change a viewpoint of acid-base reaction from matter to process

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Many students have difficulty learning acid-base concepts. The reason for this is that different acid-base models have different viewpoint, and the viewpoint of the model is mixed indiscriminately. The Arrhenius model has a material view in that the distinction between acid and base is absolute, and the Bronsted-Lowry model has a procedural view in that the distinction between acid and base is relative. In the history of science, because the layers of the Bronsted-Lowry model are piled up on the layers of the Arrhenius model, many people try to interpret the Bronsted-Lowry model as a viewpoint of the Arrhenius model. However, when a category is misconstrued, some concepts become more difficult to learn than others, which is why it is difficult to learn the Bronsted-Lowry model. On the other hand, there is a claim that only the Arrhenius model is taught to students because it is difficult to learn the Bronsted-Lowry model. Acids and bases are substances, however it must be understood in viewpoint of process because acids and bases are treated as chemical reactions at higher levels of chemistry, especially chemical equilibrium. Therefore, a new explanatory method of acid-base concept is needed to change a viewpoint from matter to process, the program to form a process-oriented view of acid-base was developed and applied to 60 high school. As a result, the understanding of the strong acid and weak acid, the understanding of the relativity of acid, the understanding of the leveling effect, and in particular, the understanding of why the precondition of aqueous solution is important in Arrhenius model were improved.

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Code: **EDU.P-503**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Effects of particle viewpoint research program on science teachers' conception of the atmosphere homogeneity

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Particle viewpoint is the most important and basic concept in the world of materials, However, many students and teachers do not have the modern particle viewpoint on the atmosphere and its homogeneity, as well. To improve this, the study program should be introduced in view of particle on the atmosphere homogeneity to the teachers who were the most influential to the students during the science class. The program was developed and trained for 26 current teachers to have the right viewpoint of scientific particle in this study. (Table 1.) The data was collected and the concept were analyzed by survey and post answers on their viewpoints and the changes. Upon the study results, significant portion of the teachers confirmed the changes into the viewpoint of modern particle concept. By doing this, it was suggested to provide the educational program in view of particle to the students and the educational places.

Table 1. Research Target Status

Classification	Grade			Year of teaching			
	1-6	7-9	10-12	0~5	6-10	11-15	Over16
Part A							
Number of teachers	13	8	5	11	4	5	6

Classification	Subjects (Elementary Teachers)		Subjects (Secondary Teachers)				
	Elementary Science	Others	Physics	Chemistry	Biology	Earth Science	Integrated Science
Part B							
Number of teachers	13	8	5	11	4	5	6



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Code: **EDU.P-504**

Area: Chemistry Education


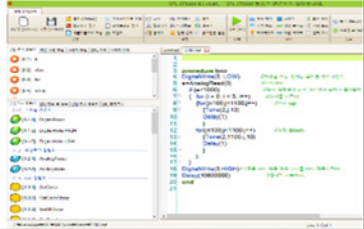
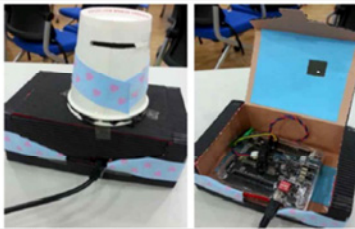
Type: Poster Presentation, Time: FRI 13:00~14:30

What did pre-service science teachers in engineering design projects learn?

Hee Jin Noh, Seounghey Paik*

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We would like to help future science teachers broaden their understanding of preparation process utilizing engineering tools at their classes. Currently, this field is barren of research although increasing interest. Therefore, this study researched about preservice science teachers (PST) who participated in engineering design project (EDP). We studied what they learned from this project. The results of the study can be summarized as follows. (1) we could not say whether the project is success or not with the success of problem solving. Learning was made although there were some failures of resolving questions. Thus, we think the project is succeed. PST could escape from a stereotype that there was no gain if they did not solve their assignments. (2) PST realized variety of possible solutions by doing EDP. The PST participating in the EDP produced fine dust measuring tools in various ways for each team. With this project, PST also could avoid from a stereotype that each problem has only one right answer. (3) PST understood students can learn concurrently science and learning, and science and engineering have similar problem-solving processes. Through this fact, PST were able to be free from another stereotype that students have to learn separately science and engineering. (4) Important discovery of this study is PST find their future prospect as teachers by themselves during EDP execution. We found PST use EDP as an opportunity of thinking their roles. To sum up, we expect EDP will promote to find identities of PST and teachers. The conclusion of this study is as follows. EDP should be further expanded in the provision of pre-service teachers in order to familiarize the PST with engineering and provide opportunities to form their identity as a teacher of the future.

		
<p>Solution 1. Measuring fine dust amount by checking luminance changing</p>	<p>Solution 2. Measuring fine dust amount by electrostatic method</p>	<p>Solution 3. Measuring fine dust amount using slide glass inside luminance changing</p>

[Figure] PSTs' various EDP problem solving method and artifact



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Code: **EDU.P-505**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Reinterpretation about the mental model of acid and base-Focusing on application of models according to Context-

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Students have a lot of difficulties in learning acid-base concept, and as a cause of confusion there is a conflict of explanation of various acid-base models. The model has a different context for each model, and the definition of the same term varies accordingly. For example, in the Arrhenius acid-base model, water can not be an acid because definition of Arrhenius acid is a substance that releases hydrogen ions in an aqueous solution. However, in the Bronsted-Lowry acid-base model, water acts as an acid against ammonia because definition of Bronsted-Lowry acid is a substance that gives hydrogen ion. However, because students can not distinguish between these different contexts, they are confused about why neutral water become an acid. So far, there have been many studies on acid-base learning and alternative concepts, but existing studies have been focused on the acid-base concept. However, this concept is based on the model, and therefore, students must develop the viewpoint of the model in order to understand the acid-base concept. Therefore, this study explores the learning process of acid-base focusing on context-appropriate model application and suggests the implication to the curriculum.

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Code: **EDU.P-506**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Supporting teaching practicum of pre-service chemistry teachers through social media

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Teaching practicum is an important opportunity for pre-service teachers to practice what they have learned from university. During 4 weeks of periods, they struggled to learn administrative things from teachers, plan and implement their own lessons, and sometimes counsel students while adapting to unfamiliar environments. Although teach-in-charge helps them to fit in, but still much help is needed. In terms of university, teaching practicum is a period when load of teaching is decreased for professors. Professors are asked to monitor and supervise their intern-teachers, but usually one time visit is enough. Pre-service teachers are quite away from university, giving help is not so easy. In this study, we built an online community on social media, and communicated during the practicum period. Graduate teachers were also invited as their mentor, and gave feedback for pre-service teachers. Pre-service teachers were asked to write some reflective journal as well as questions and requests. After practicum ends, perceptions of pre-service teachers and graduate teachers on this online mentoring on social media, and all the postings and comments were analyzed and categorized. Educational implications will be discussed.

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Code: **EDU.P-507**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Survey of Bangladeshi Science Lecturers' perception on Universal Design for Learning

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Students are different with different age, ethnicity, socioeconomic status, level of preparedness, learning English, employment and caregiver responsibilities and characteristics that effect vision, understanding capacity, language efficiency, cognitive processing, and emotions. In science classroom there are diverse learners, there is no single method of teaching that can meet the needs of all students. Instead, multiple, flexible methods of instruction are needed. But traditionally, while the teachers take class they consider the average standard of the student and that's why some of the students with disabilities can not follow the lectures properly. The reason is that all the students' perception is different as like as our finger print. But the problem can solve easily by using Universal Design for Learning (UDL) in class room. UDL is recently identified as a contemporary instructional model for promoting inclusion and equitable opportunities for diverse and struggling learners. In the developing countries like Bangladesh, research regarding science lecturers' perception on universal design for learning is limited. So, it is difficult to know how to make proper planning, implementation, and providing professional development based on Universal Design for Learning in Bangladeshi university. In this study, the Inclusive Teaching Strategies Inventory (ITSI) has been conducted to justify the university science lecturers' perceptions of UDL approaches and technologies used in classrooms. A series of MANOVA and descriptive analysis will be performed to identify predictors of these believes and actions of lecturers and the brief result of statistical analysis will be presented.

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Code: **EDU.P-508**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Analysis of Exhibits related to Chemistry in Busan National Science Museum

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The purpose of this study was to analyze the exhibits related to chemistry displayed in the science museum by exhibition techniques. I analyzed the exhibits related to chemistry displayed in the permanent exhibition hall of the Busan National Science Museum by operabilities of the exhibits, the visitors' viewing and manipulating activity types, the explanation types of the exhibits, personnel needed to operate the exhibits, and the intention of the exhibits. As a result of analyzing the chemistry-related exhibits of the Busan National Science Museum, more than 90% of them consisted of dynamic exhibits. And more than 90% of them also showed active viewing and manipulating activity type, and it was much larger than passive viewing and manipulating activity type. About 53% of active exhibits consisted of operation-exhibit 2 (including computer simulation), and 38% of them consisted of experience exhibits. All exhibits can be operated alone and about 78% of the chemistry-related exhibits consisted of hands-on exhibit.

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Code: **EDU.P-509**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Verbal Behaviors and Interactions in Processes of Making Written Test Items by Paired Think Aloud Problem Solving for Pre-service Secondary Teachers

hunsik kang

Seoul National University of Education, Korea

This study investigated verbal behaviors and interactions in processes of making written test items by paired think aloud problem solving for pre-service secondary teachers. The processes of making written test items using paired think-aloud problem solving in four small groups consisting of two pre-service chemistry teachers were recorded and transcribed. The analysis of the results revealed that 'item making' of 10 subcategories for solver's verbal behaviors were most frequently exhibited regardless of 'integration' among pedagogical content knowledge (PCK) components. The solver's 'provide', 'modify', 'require agreement', 'ask', 'agree', and 'justify' were also frequently exhibited although fewer than 'item making'. Especially, the solver's 'ask' was more frequently used in 'non-integration', whereas 'justify' was more frequently used in 'integration'. In listener's verbal behaviors consisted of 8 subcategories, 'point out', 'ask', and 'agree' were frequently exhibited regardless of 'integration'. Especially, listener's 'ask' and 'agree' were more in 'non-integration', whereas 'point out' was more in 'integration'. Many verbal interactions were analyzed to be in symmetrical type more than solver-dominant type or listener-dominant type. The symmetrical type was also more frequently exhibited in 'integration', whereas solver-dominant type was more frequently exhibited in 'non-integration'. There was little difference between 'integration' and 'non-integration' in the listener-dominant type. In 23 subcategories of the symmetrical type, 'ask-provide' and 'point out-justify' were most frequently found. Especially, 'ask-provide' was more frequently found in 'non-integration', whereas 'point out-justify' was more frequently found in 'integration'. 'Point out-modify' was the most frequent in 4 subcategories of the listener-dominant type, while 'item making-agree' in 3 subcategories of the solver-dominant type regardless of 'integration'. However, other subcategories of the three types were a little found.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: **EDU.P-510**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Some Features of Planning Lessons Using Analogies by Pre-service Secondary Science Teachers

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In this study, we investigated the features of planning lessons using analogies by pre-service secondary science teachers. Eight pre-service teachers at a college of education in Seoul participated in this study. After the workshop of instructional analogies in science education, they planned lessons using analogies. We also conducted semi-structured interviews. For the analyses, we used a revised framework from previous works which characterized the dimensions of teaching through analogies.

The analyses of the results revealed that most pre-service teachers planned to use analogies in developing lesson and to present analogs before target concepts. They also planned to explain mapping and work with analogies such as analyzing mapping, which are teacher-centered activities. Only a few pre-service teachers planned to grasp students' understanding of analogs and target concepts in order to give some feedbacks. Many planned not to explicate mapping and not to cover differences, because they thought that students could misunderstand mapping and differences could make students confused. Most planned to use videos, figures, and pictures to help students understand analogies that they presented, and some planned role-playing analogies. Educational implications of these findings are discussed.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU.P-511**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

PCK Components and Their Integrations Considered in the Processes of Developing Constructive Performance Assessment by Pre-service Secondary Chemistry Teachers

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In this study, we investigated the PCK components and their integrations considered in the processes of developing constructive performance assessment by pre-service chemistry teachers. Eight pre-service teachers participated in this study. After the workshop of theory and practice of constructivist assessment for three weeks, they developed constructive performance assessment through the planning, embodying and discussion steps. The think-aloud method was used to investigate their developing processes. Their activities were recorded and videotaped, and semi-structured interviews were also conducted. The analysis of the results revealed that the PCK component considered in the planning step showed almost the same proportions of the knowledge of assessment, instructional strategies, students, and subject matter. In the embodying step, the knowledge of assessment was most frequently used. In the discussion step, the proportions of the knowledge of assessment, instructional strategies, and students were almost the same. However, the knowledge of curriculum and the science process skill in the knowledge of subject matter were used a little throughout the developing processes. The integrations among the PCK components were found to be centered on the knowledge of instructional strategies in the planning step and the knowledge of students in the embodying step. However, the knowledge of curriculum and subject matter were hardly integrated with the other PCK components. In conclusions, emphasizing constructivist assessment in developing performance assessment could increase the quantity and quality of the integrations among PCK components. Educational implications are discussed to improve the pre-service teachers' ability to develop constructive performance assessment.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU.P-512**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Comparative study of Korean Science Education Curriculum and the United States Next Generation Science Standards(NGSS) for high school chemistry and life science connectivity

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This study examined the new biochemical content elements in revised 2015 curriculum and the revised 2009 curriculum, and compared with NGSS in the USA. The classification of biochemical content elements included in the curriculum was conducted according to the national science and technology standard classification system. As a result of the study, the number of content elements related to biochemistry decreased in integrated science and chemistry subjects, while the number of content elements covered in life sciences increased in the 2015 curriculum compared to that of 2009. Comparative analysis revealed that the achieved standards presented in the 2015 curriculum outnumbered those presented in the NGSS, but there was no significant difference in the ratio of biochemical content out of whole science subjects. Both the 2015 curriculum and NGSS offered good linkage of biochemical contents in the level of school grades(elementary – middle – high school grade). The high school science curriculum of Korean 2015 curriculum present clearer linkage of biochemical contents within science subjects than NGSS by indicating each subjects and chapters, while NGSS only presents disciplinary core ideas(DCIs). However the NGSS included summary of key biochemical concepts related to DCIs. Interestingly, the NGSS offered further linkages with biochemistry contents with non-science subjects such as English and Mathematics, possibly anticipating broader connectivity and better learning effectiveness.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: **EDU.P-513**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

Should Elementary Students Know How to Make Oxygen Gas?

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Oxygen is an essential gas for our life and very closely related to our living. The activities for making oxygen gas have been introduced in the elementary science textbook for a long time. Traditionally, we used to introduce the reaction of manganese dioxide and hydrogen peroxide to produce oxygen gas. In this study, I tried to investigate the historical changes of the activities for making oxygen gas and to introduce novel activities in the process of writing new elementary science textbook. For this purpose, I analyzed elementary science textbooks issued during the last 70 years since the establishment of the government of the Republic of Korea and examined some kinds of elementary science textbooks in the United States and Japan that have influenced Korean science education. The results of the study are as follows. First, I could not find significant change in activities for making oxygen gas in elementary science textbooks in spite of the changes in curriculum in Korea. Second, I could find activities similar to those in Korea in elementary science textbooks in Japan, but it was difficult to find relevant contents in US elementary science textbooks. Third, I found some simple and novel activities to get oxygen gas on the web. I will discuss the unnecessary of activities for making oxygen gas in elementary science in the poster presentation.

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Code: **EDU.P-514**

Area: Chemistry Education

Type: Poster Presentation, Time: FRI 13:00~14:30

The development and effect of Collaborative Problem-Solving Instruction model in science education

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This study examined the development and the effect of the Collaborative Problem-Solving for Character Competence (CoProC) instruction model within the context of secondary science education. The participant group of this study was comprised of 73 10th grade students, whom received the CoProC program. In order to assess the effect of CoProC instruction model upon participants' collaborative problem-solving skills, we implemented reflective writing practices for participants. To evaluate the program, we administered surveys that assessed the cognition of students' collaborative problem-solving. The results of collaborative problem-solving showed that the participant group has large effect size on collaborative problem-solving and social skill of collaboration, medium effect size on and cognitive skill of collaboration. Students' answers in the survey showed that the students thought the collaborative problem-solving for character competence (CoProC) activities were helpful for collaborative problem-solving. In particular, participants were able to identify those CoProC activities which targeted and improved specific sub-elements of character competence, e.g.: caring in 'Grouping and Making Rules;' caring and responsibility in 'Deciding Roles;' collaboration, communication, and respect in 'Identifying and Sharing Problems;' collaboration and responsibility in 'Designing and Conducting Inquiry;' communication, respect, positive self-image and self-regulation in 'Decision-making;' communication and honesty in 'Suggesting Solutions;' and honesty, positive self-image, and self-regulation in 'Assessment and Reflection.'

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ENVR.P-504**

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Cu/Fly ash heterostructures for enhanced catalytic reduction of p-nitrophenol as recyclable catalyst

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In this study, new Cu/fly ash (Cu/FA) heterostructure was synthesized by impregnation method to use FA as a support material for recyclable environmental catalysts. The composition and surface structure of the catalyst was characterized by X-ray diffraction (XRD) and Scanning Electron Microscope (SEM). The results demonstrated that Cu nanoparticles were well loaded on the surface of FA especially where Fe elements were present. To examine the catalytic activity of Cu/FA, we tested the reduction of p-nitrophenol (p-NP) by Cu/FA in the presence of sodium borohydride. A variety of control tests by using different catalysts (i.e., Cu/SiO₂, Cu/Al₂O₃ and Fe/SiO₂) showed that catalytic activity of monometallic catalysts (Cu and Fe) on different supports was lower than that of Cu/Fe/SiO₂. Furthermore, we prepared HCl treated FA as support materials of Cu/FA, resulting in deactivation of Cu/FA-HCl due to the leaching of surface Fe by HCl. The results obtained from our study indicate the synergetic effect of coexistence of Cu and Fe on the surface of FA. Lastly, five times recycling test showed a good reusability of Cu/FA, which can imply the potential application of non-noble metal/FA heterostructure for the treatment of wastewater containing the catalytically degradable pollutants.

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Venue: Kimdaejeung Convention Center, Gwangju

Code: ENVR.P-505

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

The Rod-shape of FCG(Full Concentration Gradient) Cathode Material with Long-Term Cycling(3000cycles) Stability for Electric Vehicles Application

Un-Hyuck Kim

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Aluminum substitution with Ni-rich cathode material is introduced into a compositionally graded cathode with average composition of $\text{Li}[\text{Ni}_{0.61}\text{Co}_{0.12}\text{Mn}_{0.27}]\text{O}_2$ (FCG61) whose Ni and Mn concentrations are designed to vary continuously within the cathode particle. The Al-substituted full concentration gradient (Al-FCG61) cathode is tested for 3000 cycles in a full-cell, mainly to gauge its viability for daily charge/discharge cycles during the service life of electric vehicles (≈ 10 years). The Al-substitution enables the Al-FCG61 cathode to maintain 84% of its initial capacity even after 3000 cycles. It is demonstrated that the Al-substitution strengthens the grain boundaries, substantiated by the mechanical strength data, thereby delaying the nucleation of microcracks at the phase boundaries which is shown to be the main reason for the cathode failure during long-term cycling. It also shows that the Al-substitution decreases the cation mixing and suppresses the deleterious formation of the secondary phase that likely initiates the microcracks. Unlike an NCA cathode, whose depth of discharge (DOD) must be limited to 60% for long-term cycling, the proposed Al-FCG61 cathode is cycled at 100% DOD for 3000 cycles to fully utilize its available capacity for maximum energy density and subsequent reduction in cost of the battery.

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Venue: Kimdaejung Convention Center, Gwangju

Code: **ENVR.P-506**

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Structural Stability of LiNiO₂ Cycled above 4.2 V

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The spherical stoichiometric LNO particle, which was composed of compactly packed was prepared by lithiation of the Ni(OH)₂ precursor and cycled at different cutoff voltages(4.1, 4.2, and 4.3V). It was demonstrated that the Li⁺ ion intercalation stability can be greatly improved through suppression of the H2 → H3 phase transition at 4.15 V during charging by limiting the upper cutoff voltage to 4.1 V. Structural damage incurred by repeated H2 → H3 phase transition was shown by TEM analysis and correlated well with the electrochemical data. Above 4.1 V, the LNO cathode was susceptible to structural damage due to microcracking due to the H2 → H3 phase transition, which led to rapid capacity fading, whereas by avoiding the H2 → H3 phase transition below 4.1 V, the cycling stability was markedly improved. As the composition of the newly developed NCM cathodes is edging toward increasingly Ni-rich compositions, the detrimental phase transition at high voltages needs be closely addressed to ensure long-term life of the NCM cathode-based battery.

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Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.P-507

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Ce-Substituted LaFeO₃ Perovskite-Type Oxides with Enhanced Catalytic Performance and Sulfur Resistance for NH₃-SCR

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We synthesized Ce-substituted LaFeO₃ perovskite-type oxides (LCFO) via Pluronic F127-assisted hydrothermal process. Obtained LCFOs exhibited several micrometer-sized spherical morphology. Crystal structure of LCFO was pure LaFeO₃ perovskite structure with small amount of cerium because lanthanum ions were perfectly substituted by cerium ions. Increasing the ratio of Ce to La ions, however, it was found that cerium oxides were formed by unsubstituted Ce ions. The catalytic properties of LCFOs were evaluated by the efficiency of selective catalytic reduction of nitric oxide with ammonia (NH₃-SCR). Pure LaFeO₃ oxide (LFO) showed poor catalytic performance for NH₃-SCR, which is consistent with previous studies. On the other hand, NO conversion efficiencies were significantly enhanced in LCFO samples, especially in pure phased LCFO. Furthermore, the LCFO catalyst with single crystal structure exhibited high resistance against SO₂ gas. This results indicated the substituted Ce ions generated new type of active sites with enhanced catalytic activity and SO₂ tolerance.

Conference Date: October 18~20, 2017

Venue: Kimdaejung Convention Center, Gwangju

Code: ENVR.P-508

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Layer-by-Layer Assembly of Graphene Oxide Nanosheets and Molecular Metal Oxides on Hematite for Solar Water Splitting

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Solar to chemical conversion, the so-called artificial photosynthesis has drawn great attention for decades as a promising solution to modern energy and environmental problems. For example, we can produce valuable chemicals (e.g., formate, synthesis gas, and methanol) from abundant carbon dioxide and water through a series of photoelectrochemical process. For the successful development of efficient and stable photosynthetic devices, it is imperative to precisely assemble various functional materials such as semiconducting materials for exciton generation, conducting materials for exciton dissociation and charge transport, and redox catalysts for target-chemical reactions. Here, we report the development of an efficient and stable photoanode for solar water oxidation by layer-by-layer assembly of cationic graphene oxide (GO) nanosheets and anionic molecular metal oxides. GO and molecular metal oxides were used as a charge-transporting layer and water oxidation catalyst, respectively, and readily deposited on hematite without alteration of their properties, according to electron microscopy and spectroscopic analysis. It was found that their sequential deposition significantly improves the photocatalytic performance and stability of hematite. The present study demonstrate the validity of layer-by-layer assembly techniques for the fabrication of electrochemical/photoelectrochemical devices and can provide a new insight for the design of novel devices.

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Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Oxidation kinetics of algal-derived taste and odor compounds during water treatment with ferrate(VI)

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Korea*

The potential of ferrate(VI) to oxidize algal-derived taste and odor (T&O) compounds during water treatment was assessed by investigating the reaction kinetics of ferrate(VI) with selected T&O compounds. Apparent second-order rate constants (k_{app}) were determined in phosphate buffered waters in the pH range of 6 - 9. The olefinic T&O compounds show an appreciable reactivity to ferrate(VI): $k_{app} = 34$ to $639 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7. The non-olefinic T&O compounds such as geosmin and 2-methylisoborneol show negligible reactivity to ferrate(VI) ($k_{app} < 0.3 \text{ M}^{-1} \text{ s}^{-1}$). The reactivity of olefinic T&O compounds toward ferrate(VI) is poorly correlated with the Taft sigma constant as a descriptor of the olefin's substituents while the high reactivity is found for the carbon double bond of alpha, beta-unsaturated carbonyl groups. The elimination rate of the olefinic T&O compounds during ferrate(VI) treatment was significantly enhanced with increasing ferrate(VI) dose, in which the enhancement was more than the model prediction that considers the ferrate(VI) reaction alone. Aldehydes were formed from the ferrate(VI) oxidation of olefinic T&O compounds indicating the double bond cleavage as one of the major oxidation pathways. Oxidation experiments in lake and river water matrixes spiked with selected T&O compounds confirmed the efficient elimination of olefinic T&O compounds.

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Code: ENVR.P-510

Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Development of a sponge-like porous structured media for removal of nitrogen and phosphorus in wastewater treatment process

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The discharge concentration of total nitrogen and total phosphorus in wastewater has been gradually strict. Recently, various techniques such as adsorption, coagulation, conventional activated sludge, membrane and advanced oxidation process have been used for the removal of nitrogen and phosphorus. Among these techniques, biological and chemical methods have been successfully applied in wastewater treatment processes. However, many wastewater treatment processes had progressed to multi-stage system because of their technical difficulty in adequately removing the nitrogen and phosphorus. In order to simultaneously remove the ammonium, nitrate and phosphorus in one stage system, in this work, we developed the sponge-like porous composite media, which was prepared by mixing calcium carbonate, magnesium oxide, sulfur and zeolite, followed by foaming with an isocyanate-based polymer. The removal efficiencies for ammonium, nitrate and phosphorus were about 64%, 75% and 90%, respectively. Our results clearly indicate that the sponge-like porous composite media can be a good alternative to satisfactorily remove the nitrogen and phosphorus in one stage system.

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Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Determination of Atmospheric Transmission from Microwave Spectrum Measurement

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Microwave spectrum from atmospheric gases is emitted by rotational transitions. The emitted radiation can be detected from the ground at defined frequencies. The shape and intensity of the spectra are modified during passing through the atmosphere. At the atmosphere, the oxygen and water vapor including liquid water influence on the microwave transfer process. The oxygen concentration in the atmosphere is well known and is stable, but the water vapor concentration changes every moment. The transmission of atmospheric microwave spectrum is also changed by water contents of the atmosphere. In this study, we will determine the atmospheric microwave transmission by using the measured microwave spectra with different path lengths. The transmission is derived from the radiative transfer equation by using three different methods which are called log-fit, least-squares fit, and chopper wheel method. And the derived transmission is also compared to the millimeter propagation model. "This work is financially supported by Korea Ministry of Environment(MOE) as 「Graduate School specialized in Climate Change」."

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Type: Poster Presentation, Time: THU 11:00~12:30

Amalgamation of mercury by bimetallic pumice-supported nanoscale zero-valent iron

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Korea*

The aim of this study is to synthesize environmentally friendly and economically favorable bimetallic pumice-supported nanoscale zero-valent iron (p-nZVI) for Hg removal in contaminated groundwater. Bimetallic p-nZVI particles were synthesized using Ni or Cu (0.1% w/w) as a secondary metal and pumice as a supporting material with a 50:1 or 25:1 pumice to Fe ratio. After 5 minutes of reaction with 250 nM Hg(II), Hg removal efficiency of bare p-nZVI was 71% for 50:1 and 82% for 25:1 pumice to Fe ratio, whereas that of Ni-coated p-nZVI increased to 94% for 50:1 and 95% for 25:1 ratio. When Cu was used as a secondary metal, Hg removal efficiency was also increased to 93% for 50:1 and 96% for 25:1 ratio. In the same reaction, the ratio of gaseous elemental Hg, Hg(0), normalized to initial Hg(II) for bare p-nZVI was 5.9% for 50:1 and 3.6% for 25:1 ratio, and these ratios decreased to 1.0% for 50:1 and 1.4% for 25:1 when Ni-coated p-nZVI was reacted with Hg(II). Decreases in Hg(0) were also found for Cu-coated p-nZVI: 0.75% for 50:1 and 1.2% for 25:1 ratio. These low ratios of Hg(0) to Hg(II) are explained by amalgamation of Hg(0) with Ni and Cu on the bimetallic p-nZVI surface. As secondary metals react with Fe(0), they may reduce to elemental Ni and Cu by Fe(0) oxidation, and then these elemental Ni and Cu can reduce Hg(II) to Hg(0). The higher concentrations of Fe(II) as well as lower concentrations of Hg(0) were found for bimetallic p-nZVI than for bare p-nZVI, supporting suggested mechanisms. We have a plan to complete surface analyses of bimetallic p-nZVI using scanning electron microscope-energy dispersive spectroscopy (SEM-EDS), transmission electron microscope-energy dispersive spectroscopy (TEM-EDS) and X-ray diffraction (XRD) for a better understanding of the mechanisms.

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Type: Poster Presentation, Time: THU 11:00~12:30

Characterization of carbon based nanoparticle dispersion in aqueous media: Effects of ionic strength, ionic valence, and humic acid

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Abstract: In this study, the stability of carbon black nanoparticles (CB-NPs) was investigated to verify the environmental influences. The stability tests were conducted in the conditions of the solution chemistry (0.1–10 mM NaCl and 0.01–1 mM CaCl₂) and humic acid (0, 1 and 5 mg L⁻¹) in an aquatic environment. The CB-NPs suspension was observed that it is easily aggregated in NaCl solution. Especially, the rate of aggregation was increased with increasing the ionic strength. On the other hand, in the conditions of CaCl₂, CB-NPs stability was quite maintained regardless of ionic strength. This result was represented by specific adsorption of the divalent ions since the CB-NPs' zeta potential showed the trends to reverse from negative charge to positive in the range of selected ionic strength. It was observed that humic acid greatly influences the stability of the CB-NPs. In particular, the stability of CB-NPs was improved in the whole range of ionic strengths of NaCl as well as of CaCl₂. To confirm the results of stability test in aqueous system, the interaction energy between CB-NPs was estimated under all conditions by applying the Derjaguin–Landau–Verwey–Overbeek (DLVO) theory. Furthermore, stability of CB-NPs is ascribed to the steric repulsive force confirmed by applying the extended DLVO theory in the presence of humic acid. **Acknowledgement:** This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2015R1D1A3A01020766), the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (2015H1C1A1035930) and Korea Energy and Mineral Resources Engineering Program (KEMREP).

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Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Oxidation of Bisphenol A by activated persulfate using Iron(II) entrapped chitosan/alginate substrate

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The oxidative ability of persulfate (PS) has been used to effectively treat a wide range of environmental contaminants. A novel Fe(II) containing chitosan/alginate composite (Fe-Chitoal) was prepared by the simple cross-linking reaction for the activation of PS to degrade bisphenol A (BPA). The prepared Fe-Chitoal was characterized by SEM, EDX, FT-IR and XPS. The result indicated that the Fe was imprinted successfully into the composite. The Fe(II) (0.35 mM) was released from Chitoal (1g/L) without PS and Fe(III) was re-adsorbed after reaction with PS. Higher removal efficiency for BPA was obtained with PS/Fe-Chitoal than using homogeneous Fe(II) with PS. Effects of different experimental conditions like PS and Fe-Chitoal dosages, pH and anions (Cl⁻, SO₄²⁻, NO₃⁻, HCO₃⁻) on the removal of BPA were investigated. The removal increased as the PS and Fe-Chitoal dosage increased and high efficiency was maintained in the pH range of 2-10 and decreased dramatically at pH 12. The removal efficiency was also maintained with 100 mM of high anion concentration. The main mechanism of PS/Fe-Chitoal was producing radicals such as ·OH and SO₄•⁻.

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Area: Environmental Energy

Type: Poster Presentation, Time: THU 11:00~12:30

Degradation of pharmaceuticals in polluted waters by electrochemical persulfate activation using iron electrodes

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Carbamazepine (CBZ) and nalidixic acid (NAL) are pharmaceuticals that were frequently detected in wastewater effluent and surface water due to their poor removal in water treatment plants. Although electrochemical treatments show a great promise in treating the pharmaceuticals, the large scale-up is still limited by high electrode cost and maintenance. In this study, we proposed iron electrodes for the electrochemically activated persulfate (EPS) removal of CBZ and NAL in a simulated wastewater effluent. Remarkably higher CBZ and NAL efficiencies were observed in EPS compared to persulfate and electrocoagulation alone. The CBZ and NAL removal efficiencies drastically increased with increases in persulfate dosage and applied current. Both hydroxyl ($\text{HO}\cdot$) and sulfate radicals ($\text{SO}_4\cdot^-$) contributed to the oxidation of CBZ and NAL with the former being the dominant species. The presence of chloride and bromide ions dramatically increased the removal of CBZ but not NAL, probably due to the selectivity of generated reactive halide species. Nitrate also enhanced CBZ and NAL degradation while ammonium did not significantly affect pharmaceutical removal. Humic acid was detrimental to CBZ and NAL removal. Other pharmaceuticals such as hydrochlorothiazide and diclofenac were also successfully eliminated by EPS. Our results clearly demonstrated that EPS could be a promising approach in the removal of recalcitrant pharmaceuticals in various wastewater. Studies on the transformation products of target pharmaceuticals, and EPS application in real field waters are currently underway.

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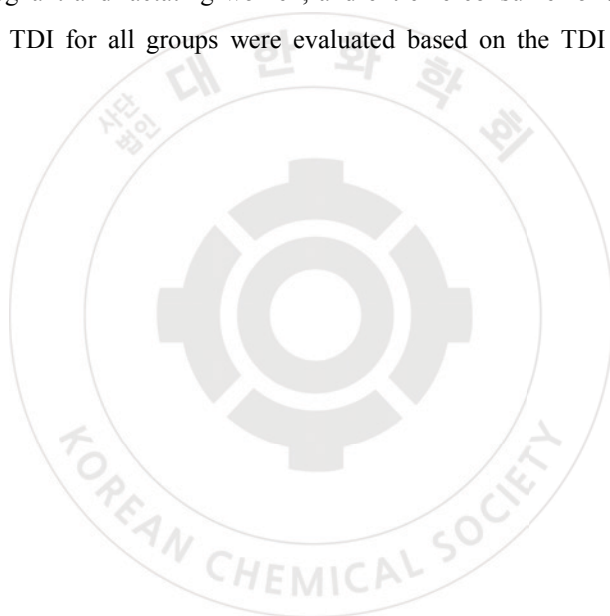
Risk assessment of PCDD/Fs and DL-PCBs in Korean population

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Various contaminants have persisted in environmental matrices and affected to ecosystem through the food chain from their sources to human. Especially, the concerned contaminants, emitted by human activity and industrial use, have been studied for their fate and estimated dietary intakes such as polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), dioxin-like polychlorinated biphenyls (DL-PCBs). Polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) and polychlorinated biphenyls (PCBs) are representative registered initial persistent organic pollutants (POPs) in the Stockholm Convention, and accumulates through food consumption. Twenty-nine congeners among PCDD/Fs and DL-PCBs are concerned due to their high toxicity. Therefore, World Health Organization (WHO) has set toxic equivalency factor (TEF) value and managed for reducing of exposure (van den, B. et al., 2006). Since both PCDD/Fs and DL-PCBs have similar toxic properties, their exposure though food consumption are managed by integrated tolerable daily intake (TDI) (Becher, G. et al., 2004). In this study, we investigated to evaluate the risk of PCDD/Fs and DL-PCBs among 2410 cases of 257 food items which are most consumed in Korea. This project was suggested by Ministry of Food and Drug Safety (MFDS) in Korea government as the largest scale monitoring that has been attempted to date. As a result of the risk assessment for the general population, we have examined whether the overall exposure can be estimated based on only the highest exposure contribution items group. These results were calculated that we can estimate the approximate exposure by monitoring only the highest exposure contribution items group instead of the large scale monitoring such as this study. Over the evaluation of only the general population, the dietary intake for each age group was separately assessed for the risk of subgroups. In particular, we considered the information of risk assessment through the calculation of dietary intake for infants and pregnant women that might be vulnerable to toxic exposure. In general, POPs such as PCDD/Fs and DL-PCBs are mainly detected in fishery products

including fish and shellfish. In this study, the levels of PCDD/Fs and DL-PCBs were in order of fishery, meat, processed and agricultural products. Fishery products were shown high concentrations in other previous studies (Shin, E.-s. et al., 2016). These results were due to the fate and characteristics of PCDD/Fs and DL-PCBs in the environment. PCDD/Fs and DL-PCBs are first introduced into the aquatic environment after they are released into the environment. And it can be attached to sediment and then dissolves into the aquatic ecosystem through decomposition, diffusion and resuspension. In land ecosystems, these compounds can be accumulated preferentially fat tissue in livestock over a long period of time. Moreover, PCDD/FS and DL-PCBs would be detected in the obtained milk and egg from contaminated livestock. However, the agricultural products which have very low fat contents showed the low levels of PCDD/Fs and DL-PCBs because the high Kow value of these compounds and hydrophobic property. The risk assessment for PCDD/Fs and DL-PCBs were estimated based on their concentration and food intake in populations. In addition, the exposure levels of the PCDD/Fs and DL-PCBs to populations were calculated by considering of the average dietary habits and body weight of the specific subgroup (e.g., age, pregnant and lactating women, and extreme consumer of 95 percentile). The daily intake and risk against TDI for all groups were evaluated based on the TDI in WHO (4 pg-TEQ/kg b.w./day).



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Influence of exposure to perfluoroalkyl substances (PFASs) on the Korean general population: 10-year trend and health effects

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This study demonstrated the 10-year trend of 13 perfluoroalkyl substances (PFASs) in serum samples of 786 adults living in Seoul, Korea. PFAS levels began to gradually increase in 2006 and then decreased starting in 2013. We found that PFAS levels were higher in males than in females and exhibited positive correlations with age. Whereas PFASs were not significantly correlated with body mass index, we observed positive correlations with total cholesterol, low-density lipoprotein cholesterol, and triglyceride and negative correlations with high-density lipoprotein cholesterol. In particular, uric acid and free thyroxine (fT4) showed positive correlations with major congeners. Inconsistent correlations were confirmed between thyroid stimulating hormone and PFASs. We demonstrated significant correlations with fT4 and perfluorononanoic acid (PFNA), perfluorohexane sulfonate (PFHxS), and perfluorodecanoic acid (PFDA). PFHxS and perfluorododecanoic acid (PFDoDA) levels showed significant differences between participants with and without diabetes. In addition, principal component analysis suggested that there might be differences in disease manifestation based on the congener distribution of PFASs. This was the longest and largest scale study to date, as well as the first on the temporal trends of 13 PFAS congeners in serum samples obtained from the Korean general population.

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Dietary exposure to decabromodiphenyl others from fishery products in Korea

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Currently, deca-brominated diphenyl ether (deca-BDE) has been included in the list of proposed chemicals under the Stockholm Convention while some other congeners (tetra-, penta-, hexa-bromodiphenyl other) were banned a few years ago. They had been produced and utilized widely until the early 21st century due to the presumption to be less toxic than lower brominated congeners. Nowadays, their bioaccumulation in the food chain and chronic toxicity has led to the proliferation of food matrices analyses. However, there are still limited reports related to this subject owing to less universal interest. Herein, seventy-five marine samples from various fish and shellfish were selected and analyzed using gas chromatography coupled to high-resolution mass spectroscopy to monitoring deca-BDE contamination. The primitive concentration of deca-DBE and the average food consumption of Korean general population, which referred to Korea National Health and Nutrition Examination Survey were used to estimate the dietary intake of this contaminants. The ultimate aim of this study is gaining an understanding of the health risk causing by daily dietary exposure of deca-BDE.

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Enhanced Hole Mobility on Electrochemically Synthesized p-type CuAlO₂ Photoelectrodes for Efficient Solar Hydrogen Production

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Delafossite CuAlO₂ photoelectrodes are synthesized via an electrodeposition of Cu(II) and Al(III) onto transparent conducting oxide (TCO) substrates in water and dimethylsulfoxide (DMSO) solvents followed by annealing in air and Ar. Optimized CuAlO₂ electrodes (synthesized in DMSO and annealed in Air) possess the suitable energetics for H₂ production under sunlight (optical bandgap of ~1.4 eV and conduction band level of ~0.24 VRHE). They exhibit the photocurrent onset potential of ~+0.9 VRHE along with the Faradaic efficiency of ~70% at +0.3 VRHE in alkaline solution (1 M KOH) under simulated sunlight (AM 1.5; 100 mW·cm²). Addition of sacrificial hole scavengers significantly improves the PEC performance of CuAlO₂ by a factor of 8 along with the faradaic efficiency of ~100%. This indicates that the hole transfer limits overall PEC performance. This challenge is addressed by employing a ~150 nm-thick Au film-coated TCO substrate for CuAlO₂ deposition. In the absence of the hole scavengers, the H₂ production with the Au-underlayer CuAlO₂ photoelectrode (Au/CuAlO₂) was three-fold higher than that with bare CuAlO₂, while the Faradaic efficiencies at +0.3 and +0.55 VRHE were ~100%. This work was financially supported by the Korea Ministry of Environment as Waste to Energy Recycling Human Resource Development Project (YL-WE-17-001), and Nano-Material Technology Development Program (NRF-2016M3A7B4908169).

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Continuous Removal of Heavy Metals by Coupling a Microbial Fuel Cell and a Microbial Electrolysis Cell

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The main objective of this study was to find the feasibility of continuous removal of mixed heavy metal ions from wastewater by coupling a microbial fuel cell (MFC) and a microbial electrolysis cell (MEC) in a continuous mode. This research focused on a mixture of chromium (VI) ions, zinc (II) ions, copper (II) ions, and nickel (II) ions, as a typical plating solution, to be removed using the MFC-MEC coupled system. The electrode material was graphite felt. To compare parameters the system was also run in a batch. In the batch mode, the effects of Cr (VI) initial concentration on removal efficiency of Zn (II) and Ni (II) in MEC has been first studied. The initial concentrations of Cr(VI), Cu(II), Ni(II), and Zn(II) were all 10 ppm in MFC, and the concentrations of Ni(II) and Zn(II) were 10 ppm in MEC. As Cr(VI) concentration increased from 10 ppm to 100 ppm, the voltage supply to MEC was increased, and Ni(II) and Zn(II) reduction rate was also increased. EIS has been applied to investigate the effect of experimental conditions on electrochemical reactions. The impedance of different Cr(VI) concentrations from 10 ppm to 100 ppm in MFCs showed that, compared with low initial Cr(VI) concentrations, higher initial Cr(VI) concentrations exhibited much lower resistance (Ohmic resistance; 19.3 ~ 13.4 ohms, charge transfer resistance; 28.2 ~ 21.5 ohms), and thus the MFCs were able to deliver more power toward MEC. The initial Cr(VI) concentration increase increased power generation by both increasing the cathode potential and decreasing the resistance of MFC. A typical current density and power density at the maximum power point were 1.08 Am⁻² and 863 mWm⁻², respectively. The typical removal efficiency for chromium ion by reduction of Cr (VI) in the MFC was in the range of 96.9% ~ 100% for 10 ppm after 8 hours. That of Cu(II) in MFC was only in the range of 29.0% ~ 29.7% for 10 ppm. On the other hand, the removal efficiencies of Ni(II) and Zn(II) in the MEC were in the range of 55.0% ~ 59.9% and 76.2% ~ 77.6% for 10 ppm, respectively. The removal efficiencies of Zn(II) and Ni(II) in the MEC were slowly increased with the initial concentration of Cr(VI) in the MFC increased. In the continuous mode, effects

of the hydraulic retention time (HRT from 2h to 12h) on the removal efficiency of 10 ppm solution have been studied. HRT had a little impact on removal efficiency of each ions. The removal efficiencies were 55.0% ~ 78.5% for Cr(VI), 30.6% ~ 32.4% for Cu(II), 55.0% ~ 59.0% for Ni(II), and 75.3% ~ 75.8% for Zn(II), respectively. Even if the initial concentration of Cr(VI) significantly changed, the other three ions showed only a little change as HRT increased.



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Study on Electrical Energy Storage System for Supplying with Environmental System

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Among the various conducting polymers, polyaniline (PANI) has received a lot of attention due to their high conductivity, good redox reversibility and environmental stability. To explore a cheap and durable power source for environmental use, polyaniline was prepared by chemical polymerization in an aqueous solution, and was tested as the cathode of a zinc-polyaniline battery with electrolyte containing 0.25 M ZnCl₂, 0.5 M NH₄Cl, 0.4 M H₃BO₃ (pH 4.0). The zinc-polyaniline battery was charged and discharged at a constant current. During the charging and discharging process, lead metal increased performance more than cadmium metal because of increasing overvoltage for the reduction of H⁺ ions in the electrolyte. When the lead metal ion concentration was 20 ppm, zinc metal could be protected from corrosion in the aqueous acidic electrolyte. And the lead metal could improve the specific capacity of the zinc-polyaniline battery. The maximum specific capacity of 100.0 mAh/g and the coulombic efficiency of 140.1% were achieved, respectively. The battery energy efficiency was calculated to be at least 97.0%.

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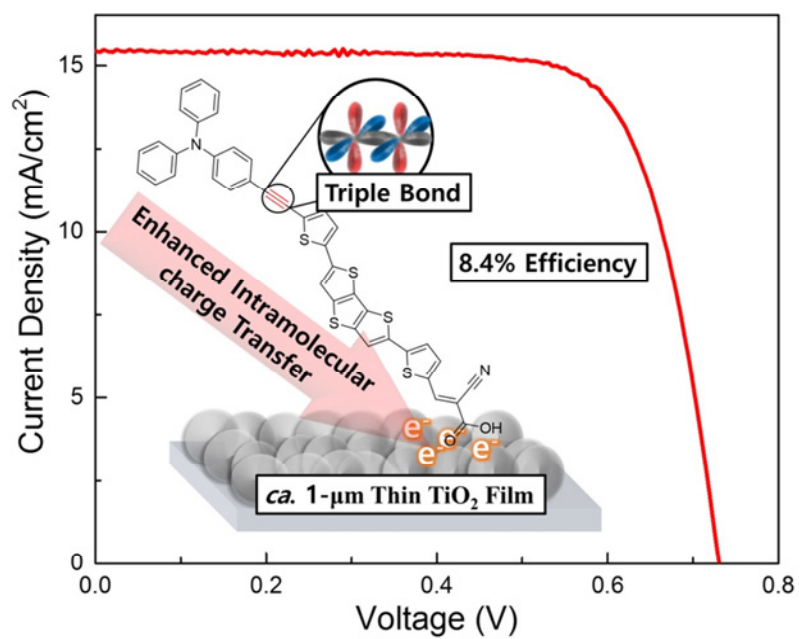
Molecular engineering for Enhanced Charge Transfer in Thin Film Photoanode

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For the commercialization of flexible dye sensitized solar cells (DSCs), to achieve high performance from a thin TiO₂ active layer (~1- μm) is indispensable because of mechanical stability and low cost fabrication. Molecular engineering of sensitizers plays a key role in the performance of thin film DSCs as the following strategies: (1) planarity for high extinction coefficients, (2) low aggregation to prevent the self-quenching of photo-excited excitons, and (3) strong intramolecular charge transfer (ICT) for efficient charge injection and broad absorption. Therefore, we developed the three types of dithieno[3,2-*b*;2',3'-*d*]thiophene (DTT)-based organic sensitizers for high-performance thin photoactive TiO₂ films and investigate the different types of bonding between the triarylamine electron donor and the conjugated DTT π-bridge by the introduction of single (S-DAHTDTT), double (D-DAHTDTT), and triple bonds (T-DAHTDTT). As a result, with only 1.3-μm transparent and 2.5-μm TiO₂ scattering layers, the triple bond sensitizer (T-DAHTDTT) shows the highest power conversion efficiency ($\eta = 8.4\%$; $V_{OC} = 0.73$ V, $J_{SC} = 15.4$ mA·cm⁻² and $FF = 0.75$) in an iodine electrolyte system under one solar illumination (AM 1.5, 1000 W·m⁻²), followed by the single bond sensitizer (S-DAHTDTT) ($\eta = 7.6\%$) and the double bond sensitizer (D-DAHTDTT) ($\eta = 6.4\%$). In this study, we suggests that the triple bond can increase the performance of DSC with a thin photoactive film by enhancing not only J_{SC} through improved ICT, but also V_{OC} through the evenly distributed sensitizer surface coverage. We analyzed these correlation mainly in terms of charge injection efficiency, level of photo-charge storage, and charge transport kinetics.



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Heterogeneous Fenton-like degradation using NTA chelated manganese ferrite

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Some chelating agents can make heterogeneous Fenton reactions faster, as well as homogeneous Fenton reactions. However, the whole mechanism of the enhanced heterogeneous Fenton reactions is still unclear, due to the coexistence of homogeneous and heterogeneous reactions. In the present work, nitrilotriacetic acid (NTA) was introduced to study the role of the chelating agent in the oxidation of diclofenac in manganese ferrite (MnFe₂O₄) system. Ferrite has similar structure with magnetite (Fe₃O₄), which Fe²⁺ sites were substituted to other metal cations. The presence of some metals in the ferrite structure strongly increased the rate of H₂O₂ decomposition and the oxidation of the organic molecules. Especially, homogeneous Mn²⁺-mediated Fenton-like process based on Fe(III)-NTA complex that is efficient at circumneutral pH range. Kinetics experiments showed that the presence of Mn²⁺ significantly enhanced the effectiveness of Fe(III)-NTA complex catalyzed Fenton-like reaction. The addition of NTA in solution accelerated diclofenac removal due to the induced homogeneous Fenton reaction by enhanced dissolution of Me²⁺ and Fe³⁺ cation. Effects of NTA surface loadings, initial H₂O₂ concentrations, initial diclofenac concentrations, calcination temperature of ferrite, and initial pH on the reaction kinetics in NTA modified ferrite/H₂O₂ system were investigated. Results showed that the surface complexed NTA (Me²⁺/Fe³⁺-NTA) inhibited H₂O₂ decomposition by competition for surface active sites, but enhanced diclofenac removal by Me²⁺/Fe³⁺-NTA was shown due to the efficient use of reactive oxygen species (ROS). Additionally, field applicability was tested in real groundwater solution, and reusability test was conducted.

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Derivation of Atmospheric Profile from Microwave Spectrum

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Monitoring the variation of the atmosphere has been performed by using several spectroscopic techniques from ultraviolet to radio-wave. The gas molecules having permanent dipole moments emits the microwaves at specific frequencies. During the propagation, its intensity and line shape is changed by the collisions with other atmospheric gases known as the collisional broadening. If we measure the atmospheric microwave spectrum, it results from the sum of the spectra emitted at each vertical layer, so we can retrieve the atmospheric profile. The profiles of stratospheric ozone and water vapor over the Seoul have been measured by the microwave radiometer of 110 GHz and 22 GHz. In this study, we will demonstrate the measured atmospheric microwave spectra and its spectral shape variation due to the meteorological condition. The vertical profiles of ozone and water vapor over the stratosphere are also shown in this study. This technique is important to study the climate change as it gives information of the upper atmosphere. Although it is known as the upper atmosphere is stable, but it means that it takes long time if its status has been changed.

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Optimization of Electrical Communication for Direct Electron Transfer of Glucose Dehydrogenase Immobilized Electrode

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Enzymatic biofuel cells are promising technology which can consume complex fuels (glucose, sucrose, etc) which is abundantly distributed in the nature, and can operate in mild pH and temperature range. The efficient electron transfer (ET) between the redox active site of the protein and the electrode surface is the main challenge for the development of high performance of enzymatic fuel cells. For the ideal ET conditions, direct ET (DET) system is needed to be constructed to exclude thermodynamic losses. So, binding stability of enzyme to electrode surface, distance of active site-electrode surface, and charge transfer resistance are the focusing issues as parameters related to DET. To optimize binding stability of enzyme to electrode and ET distance of enzyme-electrode, gold binding peptide (GBP) was site-specifically expressed via the genetic engineering of the α -subunit of glucose dehydrogenase (GDH), enabling DET between enzyme and electrode surface, as well as stable immobilization on electrode. In addition, lateral steric hindrance of neighboring enzyme is another considering point for optimization of electrical communication between enzyme and electrode surface because enzymatic steric hindrance can decrease contact area of active site on electrode and increases resistance on charge transfer processes. In this study, the influence of enzymatic steric effects on DET efficiency was investigated and proved by utilizing nano-fabricated matrix. Based on the result, it was proposed that lateral steric hinderance among enzymes should be considered as important parameter for DET and nano-fabricated electrode is necessary to control enzymatic steric effect for development of efficient enzymatic fuel cell.

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Aerobic Carbon Monoxide Dehydrogenase Immobilized on Electrode for Dissolved Carbon Monoxide Concentration Monitoring

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Syngas fermentation is a promising technology for producing bioethanol from lignocellulosic biomass. However, this technology faces several challenges, with substrate inhibition and gas-to-liquid mass transfer limitation due to low solubility of syngas components particularly carbon monoxide in the fermentation broth represent the major bottlenecks. The optimal dissolved carbon monoxide concentration in fermentation process is crucial because several microorganisms such as 'acetogens' that grow chemoautotrophically on carbon monoxide are inhibited by high dissolved carbon monoxide concentration. The aim of this study is to develop an enzyme-based biosensor for dissolved carbon monoxide monitoring which is essential for enhancing gas-to-liquid mass transfer and overcome substrate inhibition in syngas fermentation process. Carbon monoxide dehydrogenase-based biosensor is proposed for determination of dissolved carbon monoxide concentration. Carbon monoxide dehydrogenase (CODH) from the aerobic carbon monoxide utilizing carboxidotrophic eubacterium, *Hydrogenophaga pseudoflava*, unlike CODH from other aerobic carboxidobacteria produce catalytically fully competent CODH under heterotrophic condition. CODH from *Hydrogenophaga pseudoflava* is immobilized on electrode which was firstly proposed to monitor dissolved carbon monoxide. The electrochemical behaviors and electrocatalytic performance of this enzyme-based biosensor towards dissolved carbon monoxide could be used to monitor dissolved carbon monoxide concentration that will be vital for understanding, predicting and optimizing syngas fermentation process.

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Preliminary results of Mn(II) adsorption on Fe (oxyhydr)oxides in various conditions

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Manganese (Mn) is abundant in the Earth's crust as the 12th most abundant element and the 3rd most abundant transition metal. It is ubiquitous in most geological settings under a wide range of geochemical conditions such as soil, groundwater, ocean, and hydrothermal vent etc. The geochemical cycle of Mn in the environment plays an important role in the fate and transport of nutrients, toxic metals, and organic compounds by sorption or various biotic and abiotic redox processes. A redox sensitive Mn commonly exists in nature from +2 to +7. Mn(II) is principally soluble and forms a complexation with carbonate or phosphate, which is in equilibrium with insoluble solid phases (e.g., $\text{MnCO}_3(\text{s})$). Biotic and abiotic oxidation of dissolved Mn(II) consequently precipitates several Mn (oxyhydr)oxides dominantly composed of Mn(III) and Mn(IV) at various ratios. The adsorption of Mn(II) on the mineral surface is a fundamental and a crucial geochemical process to understand surface catalyzed Mn(II) oxidation and subsequent formation of various Mn (oxyhydr)oxides. However, the previous studies of Mn(II) adsorption have been generally focused on the treatment of contaminated Mn from wastewater by using several organic adsorbents (e.g., activated carbon, polyurethane). The mechanism of Mn(II) adsorption on various mineral surfaces in the environment have not been fully understood yet. In this study, the adsorption of Mn(II) on goethite ($\alpha\text{-FeOOH}$) or hematite ($\alpha\text{-Fe}_2\text{O}_3$) as a model adsorbent of Fe (oxyhydr)oxides was examined in various conditions as a function of pH, adsorbate/adsorbent ratio, and carbonate concentrations. The results of this study may provide a basic database of Mn(II) sorption on various mineral surfaces in the environment.