Plenary Lecture : **PLEN-1**

Plenary Lecture

Convention Hall 1+2, THU 13:30

Chair: Sunwoo Lee (Chonnam National University)

Selective, Catalytic Functionalization of C-H Bonds

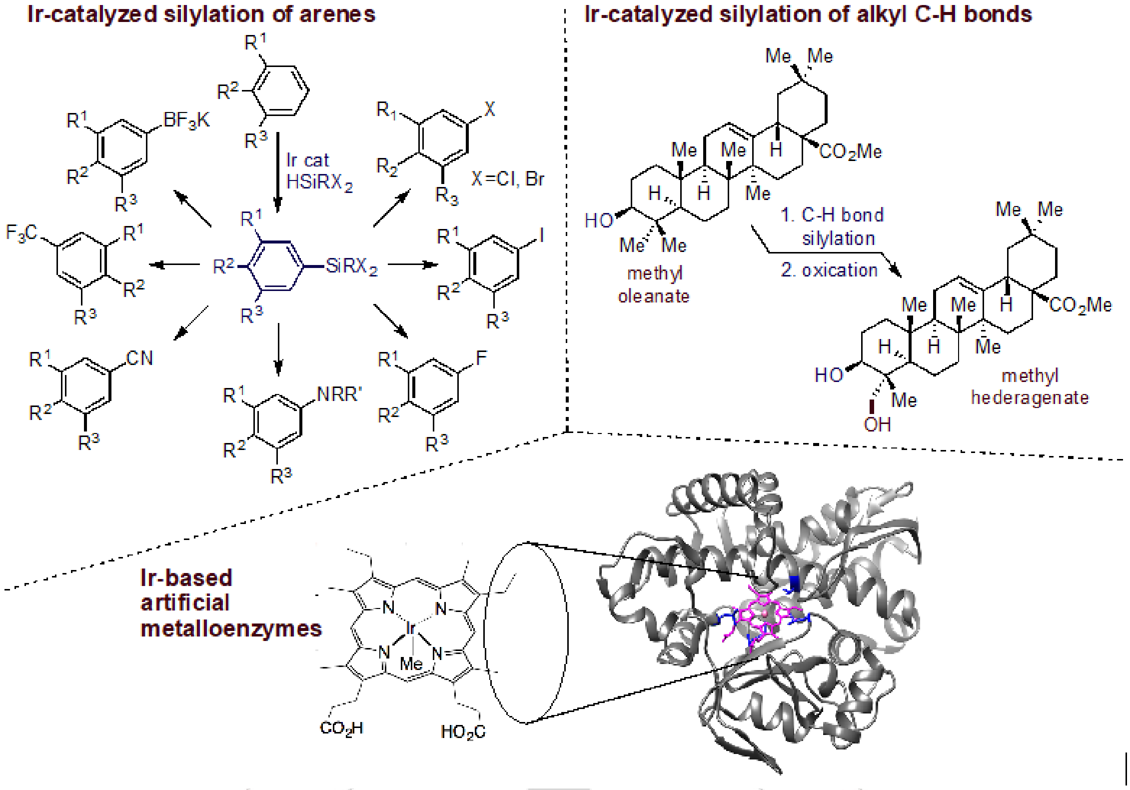
John F. Hartwig

University of California, Berkeley, CA 94720 (USA) / Division of Chemical Sciences, and Lawrence Berkeley National Laboratories, Berkeley, CA., United States

The selective introduction of functional groups into complex molecules at the positions of C-H bonds has been a longstanding challenge in catalysis. Our group has developed practical methods for the catalytic functionalization of C-H bonds with main group reagents, such as boranes and silanes, to create a comprehensive strategy to use one C-H bond functionalization process to form a range of products.

This catalysis inspired us to combine the reactions of C-H bonds catalyzed by small transition-metal complexes with the selectivity and evolutionary potential of enzymes. To do so, we have created artificial heme enzymes in which the iron of the heme has been replaced with noble metals to create catalysts for reactions that have not been catalyzed by natural or mutant heme enzymes.

This lecture will present recent directions of research in our group toward discovering selective reactions of C-H bonds catalyzed by both transition metal complexes and artificial metalloenzymes. The design and selection, as well as the intimate mechanism, of catalysts and catalytic reactions for these selective functionalization processes will be presented.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Ir cat
HSiRX2
SiRX2
X=Cl, Br
BF3K
F3C
CN
NRR'
F
I
X
Ir-catalyzed silylation of alkyl C-H bonds
methyl oleanate
1. C-H bond silylation
2. oxication
methyl hederagenate
HO
OH
CO2Me
Me
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Ir-based artificial metalloenzymes
Ir
N
Me
CO2H
HO2C

Award Lecture : **AWARD-1**
Award Lecture
Convention Hall 3, FRI 13:30
Chair: Tae-Young Kim (GIST)

Highly sensitive *in vitro* diagnostics using SERS-based microdevices: current status & future

Jaebum Choo

Department of Chemistry, Chung-Ang University, Korea

Recently, surface-enhanced Raman scattering (SERS)-based bioassay platforms have been developed for highly sensitive in vitro diagnostics. For instance, SERS-based lateral flow immunoassay (LFA) biosensor has been developed to resolve problems associated with conventional LFA strips (e.g., limits in quantitative analysis and low sensitivity). With the SERS-based LFA strip, the presence of a target antigen can be identified through a colour change in the test line. Additionally, the highly sensitive quantitative evaluation of target antigens is possible by measuring SERS signals on the test line. To verify the feasibility of the SERS-based LFA strip platform, an immunoassay of staphylococcal enterotoxin B (SEB) and a DNA assay of HIV-1 virus were performed as model reactions. The limit of detection (LOD) values are much more sensitive than those achieved with the corresponding ELISA or PCR methods. The development of SERS-based microfluidic platforms has also attracted significant recent attention in the biological sciences. SERS is a highly sensitive detection modality, with microfluidic platforms providing many advantages over microscale methods, including high analytical throughput, facile automation and reduced sample requirements. Accordingly, the integration of SERS with microfluidic platforms offers significant utility in chemical and biological experimentation. Herein, we report a fully integrated SERS-based microdroplet platform for the automatic immunoassay of specific biomarkers. These novel SERS-based assay platforms are expected to be powerful clinical tools for in vitro disease diagnosis. In this presentation, recent advances in in vitro diagnostics using optical nanosensor technology will be discussed.

Symposium : **KCS1-1**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 13:25
Chair: Seunghoon Shin (Hanyang University)

Propargylic Alcohol-Based Allene Syntheses

Shengming Ma

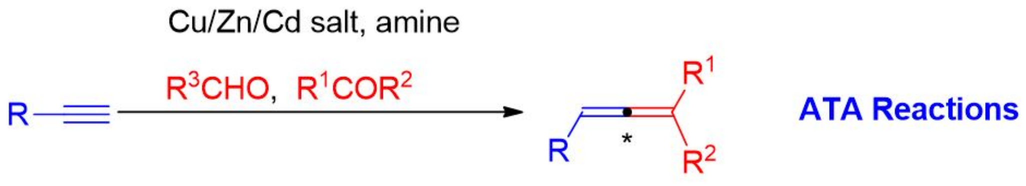
Shanghai Institute of Organic Chemistry, CAS, and Department of Chemistry, Zhejiang University and Fudan University, P. R. China, China

Abstract:

Allenes are becoming more and more important due to their potentials in organic syntheses, medicinal chemistry, and materials science, thus, development of new methodologies for the efficient syntheses of allenes from readily available chemicals are of immediate urgency. Recently, we have developed the **A**llenation of **T**erminal **A**lkynes with aldehydes or ketones reactions (ATA) for the syntheses of allenes.[1] In this lecture, I would like to share with you some of our most recent efforts towards the (enantioselective) syntheses of multi-substituted functionalized allenes using readily available racemic propargylic alcohols as the starting materials.[2-5]

References:

- Huang, S. Ma, S. *Acc. Chem. Res.*2019, **52**, 1301.
- Wang, W. Zhang, S. Ma, *J. Am. Chem. Soc.* 2013, **135**, 11517.
- Zhang, C. Huang, Y. Yuian, S. Ma, *Chem. Commun.* 2017, **53**, 12430.
- Zhang, S. Ma, S. *Chem. Commun.* 2018, **54**, 6064.
- Zheng, W. Zhang, C. Huang, Penglin Wu, H. Qian, L. Wang, Y. Guo and S. Ma *Nature Catal.* In the press.


Cu/Zn/Cd salt, amine
R3CHO, R1COR2
R
R1
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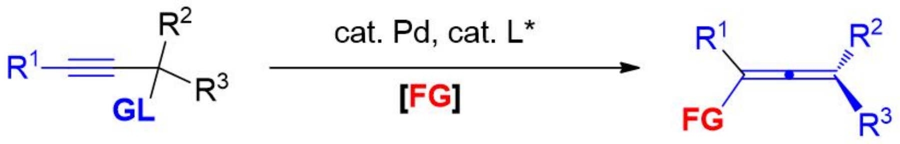
ATA Reactions


R1
R2
R3
GL
cat. Pd, cat. L*
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R1
FG
R2
R3

Symposium : **KCS1-2**

[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium

Room 301+302, WED 13:50

Chair: Seunghoon Shin (Hanyang University)

From Radical Chemistry to Dual Catalysis

Louis Fensterbank

Laboratoire de chimie théorique , Sorbonne Université, Institut Parisien de Chimie Moléculaire, France

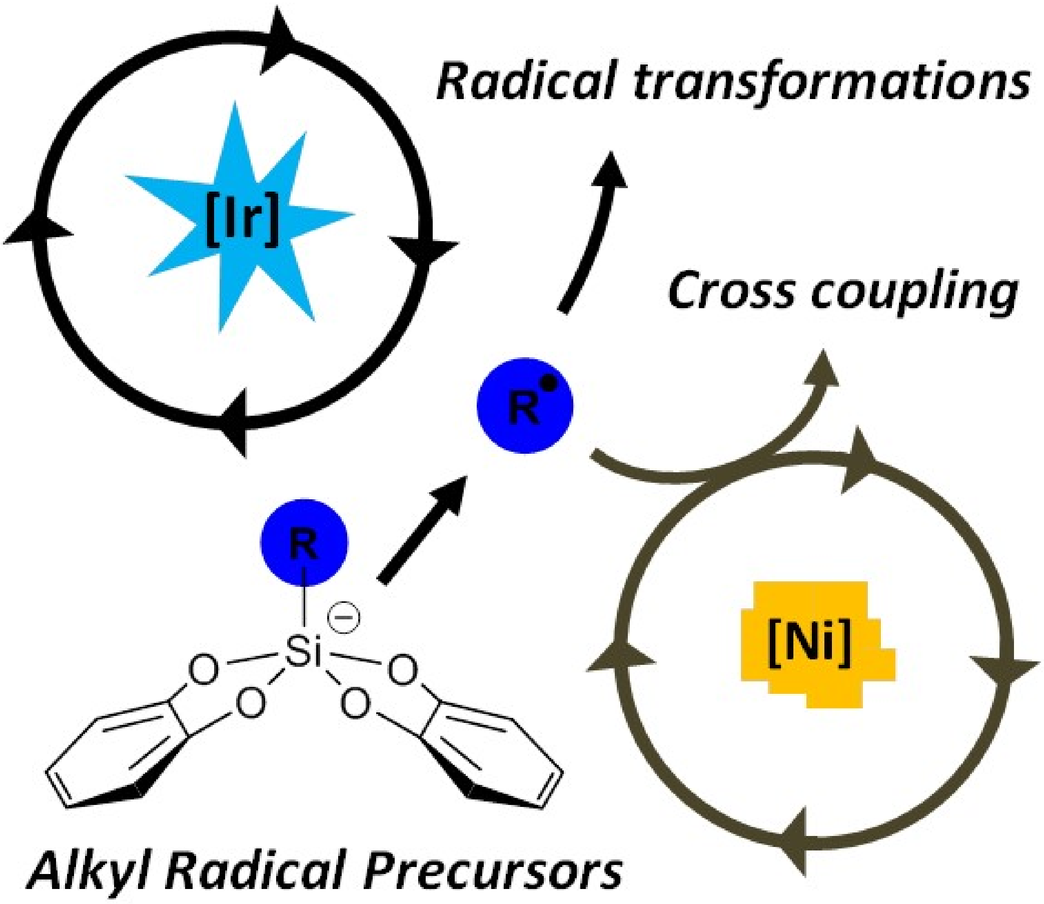
Abstract:

Over the last decade, we have been involved in the implementation of organometallic catalysis to the development of more sustainable synthetic radical chemistry. Whether relying of the use of new organometallic iron or copper complexes,[1] or photocatalytic systems,[2] we have been able to devise efficient homolytic processes with relevant applications in organic synthesis. More recently, we have introduced hypercoordinated bis-catecholato silicon compounds as versatile sources of alkyl radicals upon visible light photocatalysis. Using Ir(III) as catalytic photooxidant,[3] or an organic dye,[4] a series of alkyl radicals, including highly reactive primary ones can be generated and engaged in various intermolecular homolytic reactions. Based on cyclic voltammetry, Stern-Volmer studies and DFT calculations, a mechanism involving a single electron transfer from the silicate to the excited photocatalyst has been proposed. Finally, we have shown this oxidative photocatalyzed process can be efficiently merged with nickel-catalyzed C_{sp2}-C_{sp3} cross-coupling reactions.[3,4] Following our developments in gold catalysis[5], our recent efforts in photoredox/gold dual catalysis will also be presented.[6]

References:

1. (a) S. H. Kyne, M. Clémancey, G. Blondin, E. Derat, L. Fensterbank, A. Jutand, G. Lefèvre, C. Ollivier, C. *Organometallics* 2018, **37**, 761. (b) J. Jacquet, S. Blanchard, E. Derat, M. Desage El-Murr, L. Fensterbank *Chi. Sci.* 2016, **7**, 2030.
2. J.-P. Goddard, C. Ollivier, L. Fensterbank *Acc. Chi. Res.* 2016, **49**, 1924.

3. (a) V. Corcé, L. M.Chamoreau, E. Derat, J.-P. Goddard, C. Ollivier, L. Fensterbank *Angew. Chem. Int. Ed*. 2015, **54**, 11414. (b) A. Cartier, E. Levernier, V. Corcé, T. Fukuyama, A.-L. Dhimane, C. Ollivier, I. Ryu, L. Fensterbank *Angew. Chem. Int. Ed.* 2019, **58**, 1789.
4. C. Lévêque, L. Chenneberg, V. Corcé, C. Ollivier, L. Fensterbank *Chem. Commun.* 2016, **52**, 9877.
5. (a) Fensterbank, L.; Malacria, M. *Acc. Chem. Res.* 2014, **47**, 953. (b) Zhang, P. *et al. Chem. Cell Press* 2017, **3**, 174.
6. Z. Xia, *Nature Chem.* 2019 doi.org/10.1038/s41557-019-0295-9.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Symposium : **KCS1-3**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 14:15
Chair: Seunghoon Shin (Hanyang University)

Visible Light-Induced Site-Selective C-H Heteroarylation

Sungwoo Hong

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

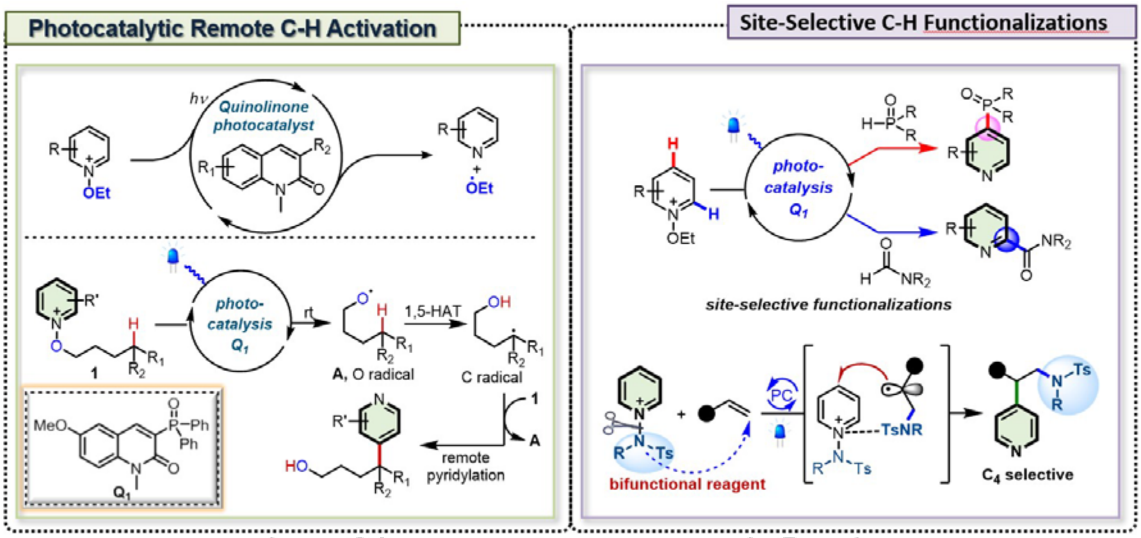
Abstract:

Our current research is focused on studying breakthrough knowledge in synthetic catalytic methods and molecular design that have a 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”. Visible-light-induced site-selective heteroarylation of remote $C(sp^3)$–H bonds has been accomplished through the design of by a photoexcited quinolinone catalyst (Q_1). This powerful transformation establishes a new synthetic method that allows for site-divergent functionalizations of pyridine derivatives driven by visible light and offers considerable advantages in both simplicity and efficiency. We expect that these new catalytic synthetic methods will be used to prepare privileged building blocks, providing opportunities for the successful implementation of fragment-based drug design (FBDD) in drug discovery research.

References:

1. K. Kim, H. Choi, D. Kang, S. Hong, S. *Org. Lett.* 2019, **21**, 3417
2. I. Kim, G. Kang, K. Lee, B. Park, D. Kang, H. Jung, Y.-T. He, M.-H. Baik, S. Hong, *J. Am. Chem. Soc.* 2019, **141**, 9239.
3. Y. Kim, K. Lee, K. G. R. Mathi, I. Kim, S. Hong, S. *Green Chem.* 2019, 21, 2082.
4. I. Kim, B. Park, G. Kang, J. Kim, H. Jung, H. Lee, M.-H. Baik, S. Hong, *Angew. Chem. Int. Ed.* 2018, **57**, 15517.

5. Y.-T. He, D. Kang, I. Kim, S. Hong, *Green Chem*. 2018, 20, 5209. K. Kim, D. Vasu, H. Im. S. Hong, *Angew. Chem. Int. Ed.* 2016, **55**, 8652.
6. Y. Moon, B. Park, I. Kim, G. Kang, S. Shin, D. Kang, M.-H. Baik, S. Hong, *Nat. Commun*. 2019, *in press*.



Symposium : **KCS1-4**

[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium

Room 301+302, WED 14:55

Chair: Bongjin Moon (Sogang University)

Diimine Multi-Purpose Platform for Chiral Ligands

Nicolai Cramer

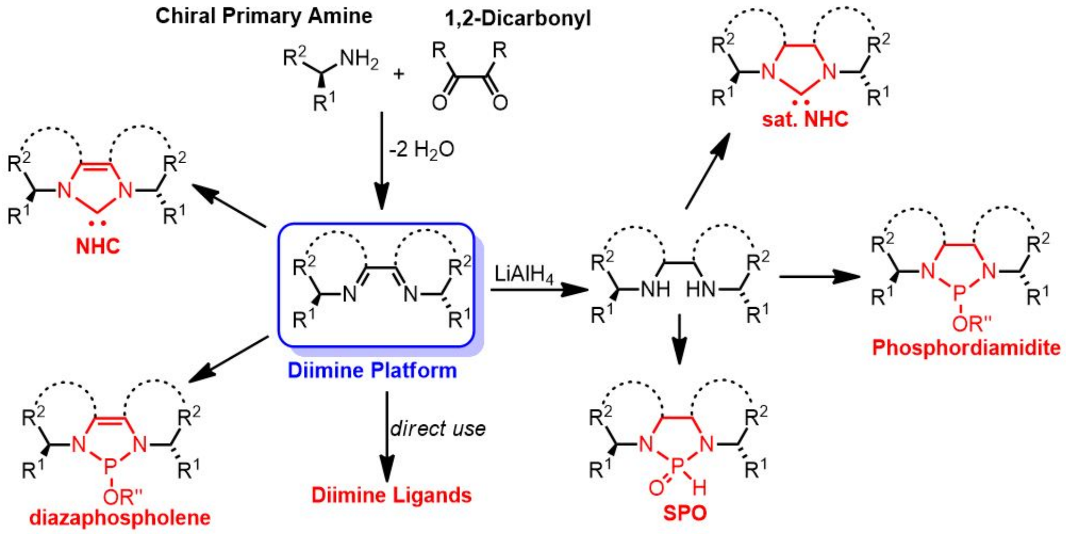
Institute of Chemical Sciences and Engineering, Laboratory of Asymmetric Catalysis and Synthesis, Switzerland

Abstract:

Reactions involving the selective activation and subsequent functionalization of C-H bonds have a high synthetic potential because of their economic and ecological benefits. Despite significant progress in addressing reactivity and selectivity issues, as well as refining mechanistic understanding of the different pathways, catalytic enantioselective transformations remain challenging. The design and development of efficient ligand systems is critical to the success these transformations. In particular, heroic "ligand total synthesis" should be avoided and highly modular approaches involving multi-purpose platform intermediates should be favored. The presentation will focus on recent developments exploiting designer amines as chirality-bearing backbones for phosphordiamidites,[1] *N*-heterocyclic carbenes[2] as well as diazaphospholenes.[3] Applications of these ligands/catalysts for a broad range of enantioselective transformation, including nickel(0)- and palladium(0)-catalyzed C-H activations will be shown.

References:

1. 1. Pedroni, N. Cramer, *J. Am. Chem. Soc.* **2017**, *139*, 12398.
2. J. Diesel, A. Finogenova, N. Cramer, *J. Am. Chem. Soc.* **2018**, *140*, 4489.
3. S. Miaskiewicz, J. H. Reed, P. A. Donets, C. C. Oliveira, N. Cramer, *Angew. Chem. Int. Ed.* **2018**, *57*, 4039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Symposium : **KCS1-5**

[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium

Room 301+302, WED 15:20

Chair: Bongjin Moon (Sogang University)

Understanding Photoexcited States of Functional Organic Materials

Lichang Wang

Department of Chemistry and Biochemistry, Southern Illinois University, United States

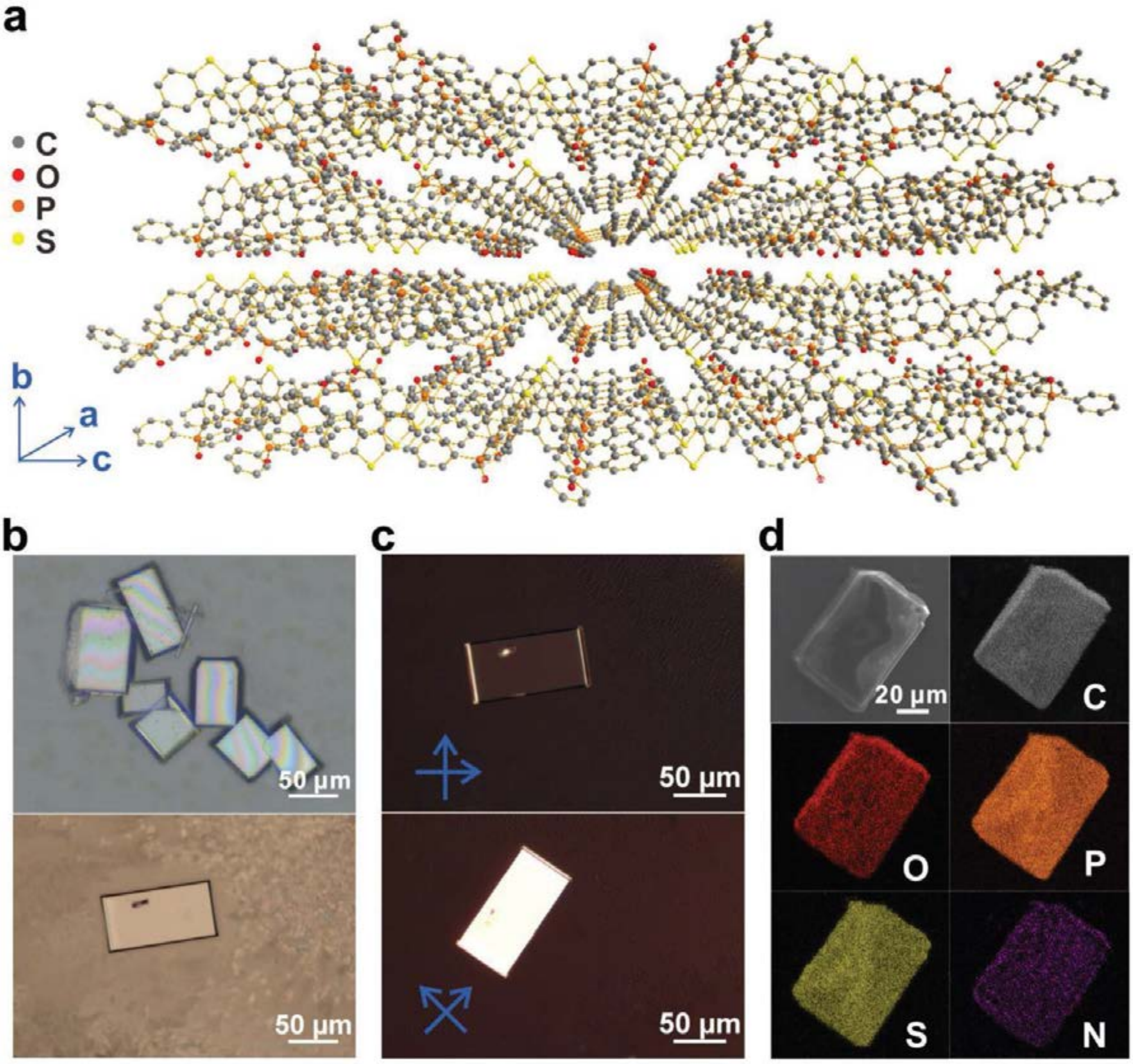
Abstract:

Understanding the correlation between photophysical properties, including excitons being generated or relaxation processes of the excited electrons, of organic materials is essential to design functional organic materials with desired performance. The functional organic materials of our interest include small molecule based photovoltaics[1] and long-persistent luminescence materials[2] (see the picture as an example).

In this presentation we will discuss the findings we have recently made with special focus on (1) the computational techniques we developed to study excitons of molecules; (2) the results of joint experimental and computational studies of excited states in a series organic small molecules and their aggregates.

References:

1. 1. Sun, P. Li, D. Liu, T. Wang, W. Li, W. Hu, L. Wang and X. Zhou, *J. . Photochem. Photobio. A: Chem.* 2019, **368**, 233.
2. J. Han, W. Feng, D. Y. Muleta, C.N. Bridgmohan, Y. Dang, G. Xie, H. Zhang, X. Zhou, W. Li, L. Wang, D. Liu, Y. Dang, T. Wang and W. Hu, *Adv. Funct. Mater.* 2019, **29**, 190250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Symposium : **KCS1-6**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 15:45
Chair: Bongjin Moon (Sogang University)

Porphyrin-based Supramolecular Nano-architectures

Woo-Dong Jang

Department of Chemistry, Yonsei University, Korea

Abstract: Porphyrins are essential pigments in biological systems. Porphyrins and chlorophylls are often self-assembled into nanoscale superstructures to perform many essential functions, such as light harvesting and electron transport. The crystal structure of the light-harvesting antenna complexes (LHC) in purple photosynthetic bacteria shows the presence of a highly symmetric wheel-like supramolecular architecture involving a large number of bacteriochlorophyll pigments. From the inspiration of the natural light harvesting systems, a variety of porphyrin-based nanoarchitectures, such as nanofibers, nanosheets, nanoparticles, and nanorings have been fabricated for applications in various research fields including photonics, catalysis, and electronics. The mimicry of light harvesting system is a very important subject, not only form a scientific viewpoint, but also for its possible contribution to sustainable utilization of energy resources. As mimic of natural light harvesting system, we recently have designed several porphyrin-based artificial models including porphyrin dendrmers, self-assembled nano-ring, and supramolecular receptors. In this symposium, we are going to report recent advances in our research related to the porphyrin-based supramolecular architectures. For example, porphyrin tripod containing triazole bridge showed formation of globular-shaped nanoparticles or linear fibrous supramolecular polymers, which have been further controlled their morphologies by addition of pyridyl guest molecules. These results could pave the way for mimicking biological systems where the macroscopic hierarchical assemblies arise in response to the microscopic changes of biomolecules.

References:

1. 1. Li, D. Yim, W.-D. Jang, J. Yoon, *Chem. Soc. Rev.* 2017, **46**, 2437.
2. D. Yim, J. Sung, S. Kim, J. Oh, H. Yoon, Y. M. Sung, D. Kim, W.-D. Jang, *J. Am. Chem. Soc.* 2017, **139**, 993.

3. W. T. Hadmojo, D. Yim, H. Aqoma, D. Y. Ryu, T. J. Shin, H. W. Kim, E. Hwang, W.-D. Jang, I. H. Jung, S.-Y. Jang, *Chem. Sci.* 2017, **8**, 5095.
4. H. Lee, Y.-H. Jeong, J.-H. Kim, I. Kim, E. Lee, W.-D. Jang, *J. Am. Chem. Soc.* 2015, **137**, 12394.
5. H. Yoon, J. M. Lim, H.-C. Gee, C.-H. Lee, Y.-H. Jeong, D. Kim, W.-D. Jang, *J. Am. Chem. Soc.* 2014, **136**, 1672.

Symposium : **KCS1-7**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 16:10
Chair: Bongjin Moon (Sogang University)

Planar and Contorted π-scaffolds for Organic Electronics

Frank Würthner

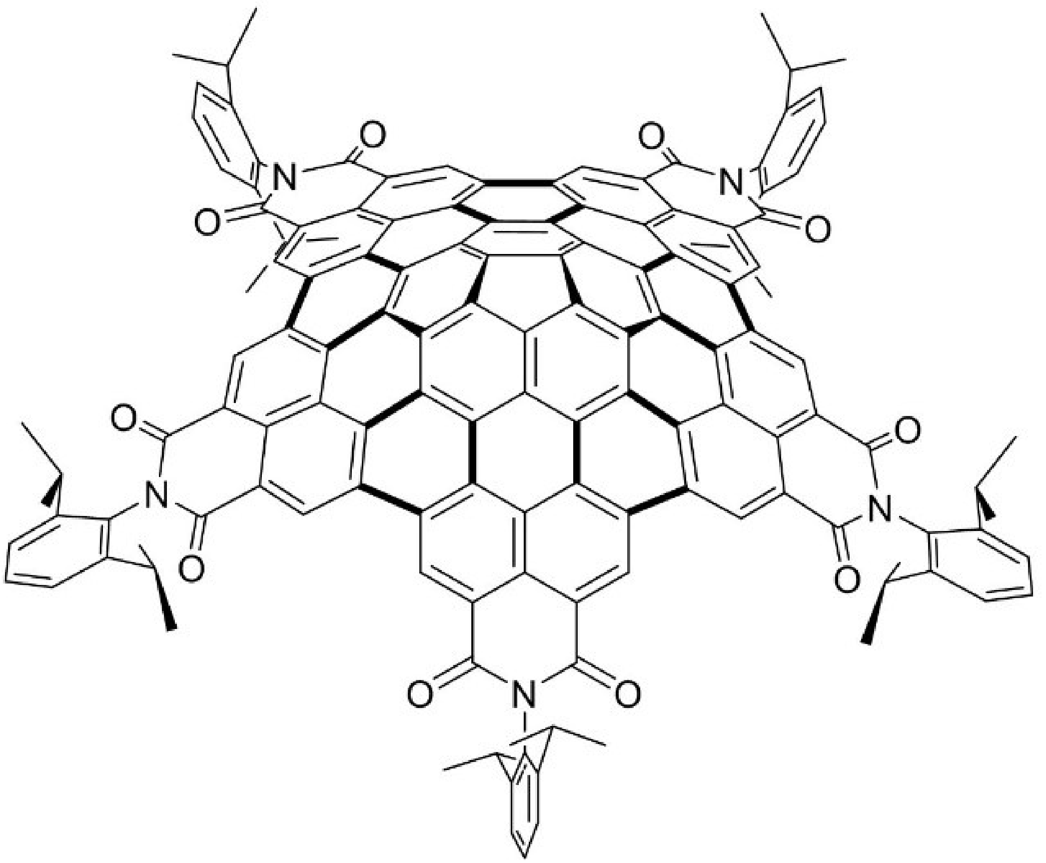
Universität Würzburg, Institut für Organische Chemie & Center for Nanosystems Chemistry, Germany

Abstract:

Despite of the fact that many functional properties of π-conjugated scaffolds only originate by the substitution of aromatic hydrocarbons with electron-donating and electron-withdrawing groups, research on larger π-scaffolds has so far been focused on the pristine subunits of graphene, carbon nanotubes or other polycyclic aromatic hydrocarbons. In contrast, driven by our ongoing interest in functional dyes and n-channel organic semiconductors,[1] we recently focused our attention on planar and contorted polycyclic aromatic hydrocarbons with low-lying LUMO levels that are realized by the incorporation of boron centers[2] or functionalization with multiple dicarboximide units[3] in the π-scaffold's periphery. Due to a lack of available synthetic methodologies towards such desirable molecules we developed a new borylation and cross-coupling-annulation cascade reactions for the synthesis of large-sized planar and contorted electron-poor π-scaffolds.[2,4] In this talk I will discuss our new synthetic methodologies and give first insights into the supramolecular and functional properties for a new class of nanosized functional π-conjugated molecules.

References:

1. M. Gsänger, D. Bialas, L. Huang, M. Stolte, F. Würthner, *Adv. Mater.* 2016, **28**, 3615.
2. J. M. Farrell, C. Mützel, D. Bialas, M. Rudolf, K. Menekse, A.-M. Krause, M. Stolte, F. Würthner, *J. Am. Chem. Soc.* 2019, **141**, 9096.
3. K. Shoyama, F. Würthner, *J. Am. Chem. Soc.* 2019, **141**, DOI: 10.1021/jacs.9b06617
4. S. Seifert, D. Schmidt, F. Würthner, *Org. Chem. Front.* 2016, **3**, 1435.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Symposium : **KCS1-8**

[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium

Room 301+302, WED 16:50

Chair: Sukwon Hong (GIST)

Carbenes as Powerful Transition Metal Surrogates

Guy Bertrand

Department of Chemistry, UCSD-CNRS Joint Research Laboratory, United States

Abstract:

It has been previously dionstrated that stable singlet electrophilic carbenes can behave as metal surrogates in the activation of small molecules and enthalpically strong E-H bonds,[1] but it was believed that these activations only proceed through an irreversible activation barrier. We will show that, as it is the case with transition metals, the steric environment can be used to promote a reductive elimination at a carbon center.[2]

Along this line, we will show that stable bicyclic (alkyl)(amino)carbenes allow for the stoichiometric carbonylation of ortho-quinones, the catalytic version being hampered by the reaction of the carbene with the quinones. However, the use of a bulky cyclic (alkyl)(amino)carbenes avoids this quenching, and thus allows for the catalytic carbonylation reaction into the corresponding cyclic carbonates.[3]

H/D exchange at formyl groups is the most direct approach for the synthesis of deuterated aldehydes. Until now, only platinum-group metal complexes were known to catalyze this transformation, with significant substrate scope limitations. We have found that mesoionic carbenes catalyze the H/D exchange of aryl, alkenyl and alkyl aldehydes in high yields and deuterium incorporation levels using deuterated methanol as an affordable D source.[4]

References:

1. G. D. Frey, V. Lavallo, B. Donnadieu, W. W. Schoeller, and G. Bertrand, *Science* 2007, **316**, 439.
2. D. R. Tolentino, S. E. Neale, C. J. Isaac, S. A. Macgregor, M. K. Whittlesey, R. Jazzar and G. Bertrand, *J. Am. Chi. Soc.* 2019, **141**, 9823.

3. E. Tomás-Mendivil, D. R. Tolentino, J. R. Peltier, R. Jazzar and G. Bertrand, *unpublished* 2019.
4. W. Liu, L. L. Zhao, M. Melaimi, L. Cao, X. Xu, J. Bouffard, G. Bertrand and X. Yan, *Chi 2019, in press*

Symposium : **KCS1-9**

[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium

Room 301+302, WED 17:15

Chair: Sukwon Hong (GIST)

Catalytic Asymmetric Addition Reaction of Heteroatom Nucleophiles to Alkoxyallene: A *De Novo* Glycosidic Bond Formation

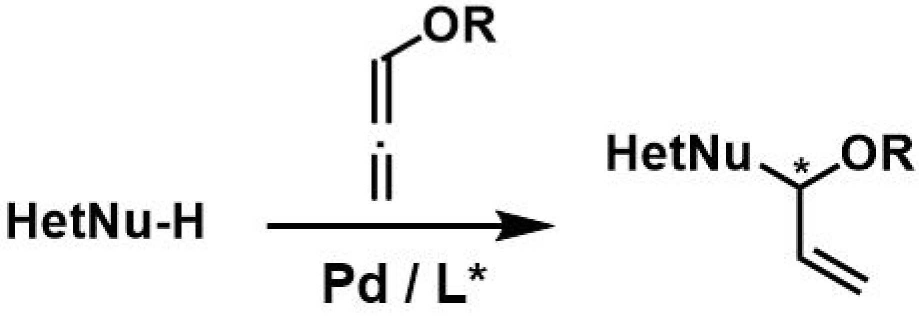
Young Ho Rhee

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

Abstract: Addition of nucleophiles to allene represents a fundamental reaction in synthetic organic chemistry. Due to the atom-efficient nature and the capability to generate stereogenic centers, this type of reaction has drawn significant attention over the last decades. Here, we report Pd-catalyzed asymmetric addition reaction of various heteratom nucleophiles to alkoxyallene. The reaction showed complete regioselectivity towards branched product formation. Numerous heteroatom nucleophiles participate well in this reaction (including alcohols, phenols, N-heterocycles, indoles, and carboxylic acids) to generate the corresponding O,O- and N,O-acetals in a stereochemically well-defined manner. Furthermore, this unique reaction was evolved into a de novo strategy towards highly useful O- and N-glycosides. In this context, application of this strategy to the synthesis of challenging targets such as deoxyoligosaccharides and ring-modified nucleosides will also be introduced.

References:

1. 1. Lee, S. Kang, D. Moon, Y. H. Rhee, *Angew. Chem. Int. Ed*., 2019, **58**, 628.
2. S. H. Jang, H. W. Kim. W. Jeong, D. Moon, Y. H. Rhee, *Org. Lett*. 2018, **4**, 1248.
3. M. Kim, S. Kang, Y. H. Rhee, *Angew. Chem. Int. Ed*., 2016, **55**, 9733.
4. W. Lim, J. Kim, Y. H. Rhee, *J. Am. Chem. Soc.* 2014, **136**, 13618.
5. 5. H. Kim, Y. H. Rhee, *J. Am. Chem. Soc*. 2012, **134**, 4011.



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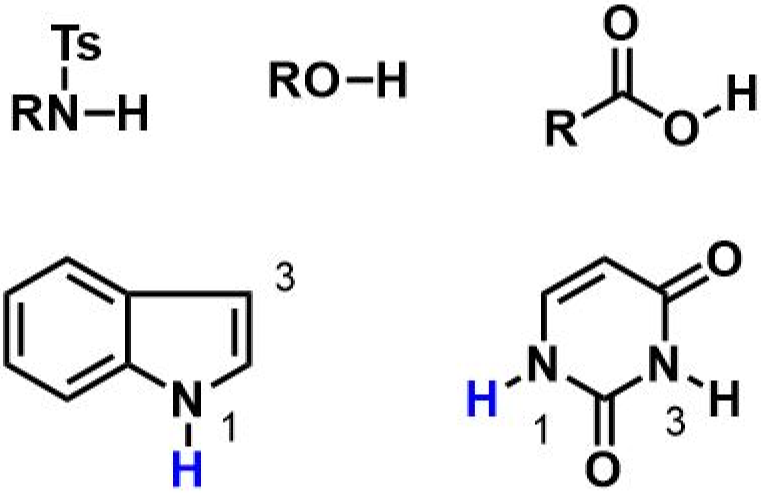

Symposium : **KCS1-10**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 17:40
Chair: Sukwon Hong (GIST)

Automation of Oligosaccharides and Glycopeptide Synthesis

Peng George Wang

Department of Chemistry, Georgia State University, United States

Abstract:

Inspired by the success of automated oligosaccharide synthesis through chemical glycosylation, a machine-driven automated system is reported here for oligosaccharides and glycopeptides synthesis through solid-phase peptide synthesis (SPPS) in organic solution and enzymatic glycosylation in aqueous solution. Thus, chemoenzymatic synthesis of oligosaccharides and glycopeptides can be obtained in an automated manner using a commercially available peptide synthesizer.[1]

References:

1. J.B. Zhang, C.C. Chen, M. R. Gadi, C. Gibbons, Y. Guo, X.F. Cao, G. Edmunds, S. Wang, D. Liu, J. Yu, L. Wen and P.G. Wang, *Angewandte Chemie International Edition* 2018, **130**, 16880.


Target molecule
Program input
Computer control
LibertyBLUE
CEM
R
Resin
+
Sugar nucleotide and enzyme
Glycosylation at 25℃
Microwave assist
Washing at 90℃
Cleaving and purification

Symposium : **KCS1-11**
[KCS-RSC Joint Symposium] The 6th Organic Chemistry Frontiers International Symposium
Room 301+302, WED 18:05
Chair: Sukwon Hong (GIST)

Small-Molecule Fluorescent Sensors for Reactive Oxygen and Reactive Nitrogen Species

Dan Yang

Morningside Laboratory for Chemical Biology and Department of Chemistry, The University of Hong Kong, Hong Kong

Abstract:

Reactive oxygen and reactive nitrogen species (ROS/RNS) play important roles in redox signaling and oxidative stress, thus serve as key regulators in human health and diseases such as cancer, inflammation, and neurodegenerative diseases.[1] By exploring new sensing strategy and responsive moiety, we have developed a series of small-molecule fluorescent sensors (HKSOX, HKPerox, HKOCl, HKOH, HKGreen/HKYellow) for highly selective and sensitive detection of superoxide, hydrogen peroxide, hypochlorous acid, hydroxyl radical and peroxynitrite, respectively.[2–8] These sensors have been widely applied in confocal imaging, flow cytometry analysis, tissue staining, and zebrafish imaging. Moreover, we have extended our sensing strategies onto other fluorescent/luminescent templates to develop more advanced probes with different excitation/emission wavelengths, ratiometric detection, and organelle-targeting properties. Our comprehensive molecular tools could be robustly applied in investigations of redox biology and medicine, facilitating the discovery of new diagnosis and therapeutics.

References:

1. C. Winterbourn, *Nat. Chi. Biol.* 2008, **4**, 278.
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124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **KCS2-1**

[KCS-SK innovation Joint Symposium] Recent Advances in Green Chemistry

Room 600A, WED 15:10

Chair: Myoung Lae Kim (SK innovation)

Homogeneous Catalysis for Sustainable Chemical Synthesis: Utilization of Methanol and Cyclopentadiene for Fine Chemicals and Polymers

Soon Hyeok Hong

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

Environmentally benign chemical syntheses that generate minimal by-products is particularly demanding for industrial processes and global society. Our research group aims to develop practical and sustainable synthetic methods through homogeneous catalysis utilizing common, versatile feedstocks. Specifically, we have explored the utilization of carbon dioxide and methanol as C1 sources for chemical synthesis, and development of highly versatile ruthenium olefin metathesis catalysts active at low temperatures, even at -60 ^{o}C. Herein, novel catalytic methods for the synthesis of ureas, formamides, and N-methyl amines utilizing methanol as a sustainable C1 reagent will be presented together with the unprecedented ring-opening metathesis polymerization of cyclopentadiene, a common feedstock from naphtha, enabled by highly active olefin metathesis catalysts developed by our group.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **KCS2-2**
[KCS-SK innovation Joint Symposium] Recent Advances in Green Chemistry
Room 600A, WED 15:55
Chair: Myoung Lae Kim (SK innovation)

Conversion of Lignin (Model) Compound and Glycerol to High-Value Chemicals

Jung Woon Yang

Department of Energy Science, Sungkyunkwan University, Korea

In recent years, mankind has become increasingly interested in biomass as natural energy resource, especially in view of the depletion of fossil fuels caused by injudicious use and related environmental impact. Among biomass materials, lignin has attracted attention because of its synthetic relevance as a potential supplier of aromatics and promising alternative source of hydrocarbon fuels. In addition, glycerol is a triol that can be generated as a by-product during the synthesis of biodiesel from vegetable oils, such as soybean and sunflower oils. However, glycerol is no longer considered a byproduct of biodiesel production and is recognized as a privileged scaffold due to its potential as a high-value carbon and oxygen source and alternative to our gradually depleting existing natural resources. We recently addressed our efforts to the design and development of the following green protocols utilizing NaO*t*Bu-O_2 system in organic synthesis: (transition) metal-free, oxidative fragmentation of lignin (model) compounds to the corresponding aromatics and conversion of glycerol to high-value chemicals such as alpha-hydroxy acid and unnatural alpha-amino acid.Individual reaction with the detailed mechanism will be present in this symposium.

Symposium : **KCS2-3**
[KCS-SK innovation Joint Symposium] Recent Advances in Green Chemistry
Room 600A, WED 16:40
Chair: Myoung Lae Kim (SK innovation)

Catalyst and process technology for producing highly valued C1 compounds from greenhouse gases

Sungho Yoon

Department of Chemistry, Chung-Ang University, Korea

The development of highly efficient and recyclable heterogeneous catalysts and their process technologies, involved in the conversion of green house gas CO2 into value added compounds, is one of the most important goals in developing climate change response technologies. Recently, we reported on a catalyst capable of producing formic acid derivatives through unprecedented carbon dioxide hydrogenation of 38,800 h-1 using ruthenium cation-treated pyridine-containing covalent triazine backbone (CTF); the catalyst [bpy-CTF-RuCl3] was used to catalyze the hydrogenation of CO2 in a very short time to produce 2.1 M of formate in aqueous solution. Furthermore, based on these heterogeneous catalysts, we are demonstrating continuous process using Tickle bed reactor to realize industrialization of this technology, which can be extended to CO2 simultaneous capture and conversion technology. This presentation will discuss this in detail.References1. ACS Catalysis, “Design Strategy toward Recyclable and Highly Efficient Heterogeneous Catalysts for the Hydrogenation of CO2 to Formate” (2018).2. Chem. Mater., “A Covalent Triazine Framework, Functionalized with Ir/N-Heterocyclic Carbene Sites, for the Efficient Hydrogenation of CO2 to Formate” (2017).

Symposium : **KCS3-1**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 14:15

Chair: Sejin Lee (Agency for Defense Development)

History of propellants in Korea and their future trends

Byoung Sun Min

Agency for Defense Development, Korea

A lot of works on solid composite propellants have been carried out since ADD was established in the early 1970s. At the beginning stage, solid composite propellants had been developed working with advanced nations. However, since the mid-1980s, ADD has started developing the solid propellants independently as well as complete localization of key materials in close-collaboration with defense industries. As a result, the level of our technologies regarding solid propellants has risen significantly and presently, some are on par with other developed countries. Lately, we have been more working on the development of solid propellants for insensitiveness to unplanned external stimuli, minimum smoke-exhaust, and eco-friendliness as well as higher performance. Along with these, we have also been studying both gelled energetic propellants with thixotropic property and fuel-rich(oxidizer-lean) solid propellants (for the air-breathing engine) which react with the air bypassed from the atmosphere during the flight of rocket for thrust modulation. As the only government organization for researching the propellants for rockets and missiles, ADD is currently striving to develop the advanced technologies related with all kinds of propellants available for rockets and missiles with more creative thinking and innovative ways of working.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **KCS3-2**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 14:40

Chair: Sejin Lee (Agency for Defense Development)

Basic Technologies for the Development of High Explosives

Hyoun Soo Kim

Agency for Defense Development, Korea

The objective of this presentation is to provide fundamental information on the subject of high explosives to chemist. Technologies for the development of high explosives are divided into 5 areas : (1)synthesis of new energetics, (2)preparation of functional explosives, (3)formulation study of plastic bonded explosives, (4)application of high explosives to munitions, (5)demilitarization process. This presentation outlines the basic technologies need to understand the high explosives.

Symposium : **KCS3-3**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 15:05

Chair: Sejin Lee (Agency for Defense Development)

Present and future of challenging military battery development

Jang-Hyeon Cho

Agency for Defense Development, Korea

Starting from the lead-acid battery developed in the mid-19th century, the battery industry has been applied to a wide range of fields such as mobile phones, automobiles, and power storage devices (ESS) since the commercialization of lithium secondary batteries in 1991, and will highlight the future industries.Although not widely known due to limited use and technical protection, military batteries have been developed for practical use one step ahead of civilian batteries.This seminar briefly introduces the development history and current development technology of military batteries used in more demanding environmental conditions (low temperature, high temperature, impact, altitude, etc.).In particular, we will introduce the special batteries used in missiles, torpedoes, future soldier systems, and share the technology.

Symposium : **KCS3-4**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 15:45

Chair: Sejin Lee (Agency for Defense Development)

Researches for Development of CBR (Chemical Biological Radiological) Defense Technology

Hyunsuk Kim

The 4th R&D Insitute - 6th Directorate, Agency for Defense Development, Korea

Chemical, biological and radiological(CBR) weapons are representative mass destruction weapons that can kill many people at low cost. Researches for development of CBR defense technology aim to effectively prevent, respond to and defend against CBR attacks and can be classified as detection, protection, decontamination, detoxification, verification and destruction. This symposium will introduce ADD's researches in the field of CBR.

Symposium : **KCS3-5**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 16:10

Chair: Sejin Lee (Agency for Defense Development)

Synthetic Biological Technology as a focal point of ADD's future R&D efforts

Juhyun Kim

IDAR of ADD, Agency for Defense Development, Korea

While tension of technology competition is rising up in the word, great powers, USA and China etc., seek for future military capabilities from Synthetic Biology, which would be emerging threats for national defense. To defend ourselves from the potential threats, the ADD puts an effort for establishing a S&T function of Synthetic Biology. That function also spans Brain scanning technology with EEG and Brain-Machine Interfacing. In addition, ROK-US defense technology cooperations are introduced to promote access to US defense S&T commuinites.

Symposium : **KCS3-6**

[Defense Science Symposium] Introduction of ADD's Researches and Future

Room 700B, WED 16:35

Chair: Sejin Lee (Agency for Defense Development)

Introduction of CMTC (Civil Military Technology Cooperation) Programs

Hyeonwoo Lee

Agency for Defense Development, Korea

This is an introduction to civil-military technical cooperation program in korea. The purpose, history, procedure, and business types of the civil-military technical cooperation program, which has been carried out since 1998, are described. Additionally, major outcomes and ongoing projects by business type are introduced.

Symposium : **KCS4-1**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 15:00
Chair: Yoon-Kyoung Cho (IBS)

Diffusion Enhancement of Catalytic Enzymes

Ah-Young Jee, Steve Granick*

Center for Soft and Living Matter, Institute for Basic Science, Korea

Too much remains speculative about how the internal dynamics of enzymes relates to catalytic function, due to lack of appropriate methods to detect millisecond time scales over sufficiently small observation windows. Here, we used super-resolution microscopy (stimulated emission-depletion fluorescence correlation spectroscopy, STED-FCS) and observe than during catalysis an active enzyme spontaneously migrate toward the direction of lower reactant (substrate) concentration using the run-and-tumble motion, a strategy similar to that of some swimming microorganisms. Experimentally, we show that enhanced enzyme mobility is generated by super-diffusive kicks generated at the substrate turnover frequency. Pursuing this idea, we have explored methods to vary systematically the turnover frequency, kcat, which defines how many substrate molecules are consumed in a given time. These results help us understand activities of enzymes, and furthermore to design and use a synthetic self-propelled swimmer relevant to "active matter".

Symposium : **KCS4-2**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 15:30
Chair: Yoon-Kyoung Cho (IBS)

Self-assembly in rotating frames of reference.

Yaroslav Sobolev, Bartosz Grzybowski[1,*]

Center for Soft and Living Matter, Institute for Basic Science, Russia
[1]*IBS Center for Soft and Living Matter / Department, Ulsan National Institute of Science and Technology, Korea*

In dynamic self-assembly, DySA, the non-equilibrium conditions are usually established by external stimuli such as time-changing light, electric or magnetic fields. At the same time, the experimental system as a whole is held stationary. In this talk, we will discuss non-equilibrium systems that depart from this conventional approach and establish non-equilibrium conditions by translating from a stationary to a moving frame of reference, with emphasis on rotating systems. Examples will be provided in which such "global" rotation drastically changes the self-assembly or even chemical processes, yielding new types of assemblies and structures.

Symposium : **KCS4-3**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 16:00
Chair: Yoon-Kyoung Cho (IBS)

Nanocrystal Conversion Chemistry within Nanosilica Confinement

<u>In Su Lee</u>

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

The extensive research performed in the past two decades has enabled to produce a range of colloidal nanocrystals mostly through solution-based procedures that generate and transform nanostructures in bulk-phase solutions containing precursors and surfactants. Unlike well-established solution-based methods, solid-state reactions, which had been at the forefront of traditional inorganic materials chemistry, are quite rarely utilized in the realm of nanomaterials; this is because of the high temperatures required for most of the solid-sate reactions, the clusters and NCs are prone to migrate through bulk reaction medium and sinter together into uncontrollable large particles. We have been pursuing the "nanospace-confined approach” to explore the use of nano-sized solid-state reaction media to carry out the syntheses and transformations of nanocrystals in a unique microenvironment; partitioning the reactants, intermediates and transition states from rest of the bulk reaction media. Such nano-confined systems have potential not only to enable efficient and selective nanocrystal-conversion chemistries but also to provide fundamental understanding pertaining to the synthetic evolution of nanostructures and transient mechanistic steps. Unique few tens of nanometer-space inside nano-confined systems offers the opportunity to observe and elucidate novel deconvoluted chemical phenomena that are impossible to investigate in bulk systems; and, comprehensive understanding of nano-confined chemistry can be implicated in explaining and controlling the macroscopic chemical behaviors. In this presentation, I will discuss the key examples of “nanospace-confined solid-state conversion approach”, which involve the novel reactions of nanocrystals within a thermally stable solid silica nanospheres to synthesize and transform complex hybrid nanocrystals with increased complexity and functionality.

Symposium : **KCS4-4**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 16:30
Chair: Yoon-Kyoung Cho (IBS)

Soft Matter Dynamics at the Nanoscale

John King

Center for Soft and Living Matter, Institute for Basic Science, Korea

The interfacial physics of complex fluids under flow remains a fundamental question in hydrodynamics. In particular, the structure and dynamics of polymers near solid walls, both at equilibrium and under flow, has received renewed interest due to the emergence of nanofluidics and confined transport. A significant challenge in the field, however, is overcoming the reliance on bulk-level measurements that average over spatial and temporal heterogeneities. Rapidly advancing microscopy and spectroscopy techniques, including super-resolution fluorescence microscopy, provide access to the spatial and temporal dimensions that often govern macroscopic structure and dynamics. This talk will introduce novel adaptations of super-resolution fluorescence microscopy and discuss the resulting experimental progress in understanding interfacial dynamics of flowing complex liquids.

Symposium : **KCS4-5**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 17:00
Chair: Yoon-Kyoung Cho (IBS)

Biomolecules-controlled Chirality in Gold Nanoparticles

Ki Tae Nam

Division of Material Engineering, Seoul National University, Korea

Chiral structure controlled at nanoscale provides a new route to achieve intriguing optical properties such as polarization control and negative refractive index. However, asymmetric structure control with nanometer precision is difficult to accomplish due to limited resolution and complex processes of conventional methods. In this regards, utilizing chirality transfer occurring at organic-inorganic materials offers viable route to overcome these limitations. Previously we developed a unique synthesis strategy that characteristic of molecule is transferred to gold nanoparticle morphology [1,2]. Based on the system, here, we demonstrated novel chiral gold nanostructures exploiting chirality transfer between peptide and high-Miller-index gold surfaces [3]. Enantioselective adsorption of peptides results in unequal development of nanoparticle surface and this asymmetric evolution leads to highly twisted chiral element in single nanoparticle making unprecedented 432 helicoid morphology. The synthesized helicoid nanoparticle showed strong optical activity (dissymmetry factor of 0.2 at 622 nm) which was substantiated by distinct transmittance color change of helicoid solution under polarized light. Modulation of peptide recognition and crystal growth enabled diverse morphological evolution and the structural alterations provided tailored optical response, such as optical activity, handedness, and resonance wavelength. We believe that our peptide directed synthesis strategy offers a truly new paradigm in chiral metamaterial fabrication and will be beneficial in the rational design of chiral nanostructures for use in novel applications. References 1.H.-E. Lee, K. D. Yang, S. M. Yoon, H.-Y. Ahn, Y. Y. Lee, H. Chang, D. H. Jeong, Y.-S. Lee, M. Y. Kim, K. T. Nam, ACS Nano, 9, 8384 (2015). 2.H.-Y. Ahn, H.-E. Lee, K. Jin, K. T. Nam, J. Mater. Chem. C, 1, 6861 (2013).3.H.-E. Lee, H.-Y. Ahn, J. Mun, Y. Y. Lee, M. Kim, N. H. Cho, K. Chang, W. S. Kim, J. S. Rho, K. T. Nam, Nature, 556, 360 (2018)

Symposium : **KCS4-6**
[IBS Symposium] Dynamic Soft and Living Matter
Room 700A, WED 17:30
Chair: Yoon-Kyoung Cho (IBS)

Harnessing tiny cell-derived vesicles

Yoon-Kyoung Cho

Center for Soft and Living Matter, Institute of Basic Science, Korea

Nano-sized extracellular vesicles (EVs) naturally secreted from cells—have emerged as promising biomarkers and potential therapeutic vehicles, but methods to manipulate them for engineering purposes remain elusive. Among the technical obstacles are the small size and surface complexity of them and the complex processing steps required, which reduce the biocompatibility of currently available methods. Here, we demonstrate our on-going research using “Lab-on-a-disc”, which applies centrifugal force to process biological fluid such as whole blood or urine to analyze cancer related biomarkers. To improve stability and to provide surface functionality, we encapsulated the EVs with a nanofilm of natural polyphenol, which could protect EVs from external aggressors such as UV-C irradiation or heat and is controllably degraded on demand. Furthermore, gold nanoparticles can be covalently attached for single-exosome level visualization. Next we introduce the microfluidic chip equipped with biologically interfaced platelet membrane-cloaked surface (PLT-Chip), which could specifically capture EVs from multiple types of cancer cell lines (prostate, lung, bladder, and breast) than the normal cell-derived EVs and clearly distinguish the plasma of cancer patients from that of normal healthy controls.

Symposium : **KCS5-1**

[KCS-KWSE Joint Symposium] The Lifetime of Woman in Chemistry: The Past, Present, and Future of Woman Chemists

Room 607, FRI 09:20

Chair: Hoi Ri Moon (UNIST)

50 Years of My Life as a Woman Chemist

Myunghyun Paik Suh

Division of Chemistry, Seoul National University, Korea

During the 50 years of my life devoting to chemistry as woman scientist, starting from March 1967 that I entered the college of Seoul National University to February 2017 that I retired from Seoul National University as a professor, there were many episodes on conducting research activities and teaching students. I would like to share some of these experiences with the audience. I will talk about what my dream was when I decided to return to Korea after obtaining the degree in US and what efforts I had made to make the dream come true. I will speak about some of the important research findings that my group has achieved in the lab, my domestic and international academic activities, unforgettable memories, and the rewarding events and regretful things that have happened in those years. In addition, I will introduce the philosophy and attitude that I have maintained while pursuing my career as a woman chemist. I will also talk about some memorable stories about my disciples and what life looks like after retirement. Finally, I would like to advise the present and next generation women chemists to pioneer their own fields and to take care of their lives so that they would less likely regret in the future.

Symposium : **KCS5-2**
[KCS-KWSE Joint Symposium] The Lifetime of Woman in Chemistry: The Past, Present, and Future of Woman Chemists
Room 607, FRI 09:50
Chair: Ha-Jin Lee (KBSI)

Life with Challenges and Passion

Mi-Sook Won

Advanced Materials Engineering, Dong-Eui University, Korea

I am an early woman researcher who retired from the government-funded Korea Basic Science Institute and is currently working at Department of Advanced Material Engineering of Dong-Eui University with the support of the National Research Foundation of Korea’s Professional Experienced Personnel Invitation Program. In this special session, “The Life Time of Woman Chemist: The past, present, and future of women chemists”, I would like to share my experiences on research activities, woman researcher's challenges, and how to overcome the difficult situation during a researcher career as a local woman scientist with active women chemists and graduate students. Through my talk, I hope that women chemists will be able to work in a better research environment, give an opportunity to change social attitude actively, and all participants can share “knowhow” and “ideas” for works and life balances, and expand chances for communication through a “mentor-mentee” relationship.

Symposium : **KCS5-3**

[KCS-KWSE Joint Symposium] The Lifetime of Woman in Chemistry: The Past, Present, and Future of Woman Chemists

Room 607, FRI 10:20

Chair: Sangwon Ko (Korea Railroad Research Institute)

The Role and Vision of Woman Chemist

Young Ok Seo

FINETECHNOLOGY CO.,LTD, Korea

During the IMF, I started a new business again. I wasn't afraid to challenge something new. I tried to do something worthwhile with a pioneering spirit. You have to know how important it is to do what you do. Also you must know your goals properly and practice them. I learned many things at the same time while teaching. I want to be called a lab master rather than a boss. There is a mind to have to run a company. You have to be a happy person for every time and keep learning in life.

Symposium : **KCS6-1**
[Laboratory Safety Education] Laboratory Safety Education for the Graduate Students
Room 602, FRI 09:00
Chair: Ik-Mo Lee (Inha University)

Guide for the Establishment of Safety Environment to Prevent Damages from Earthquakes in the Laboratories of Educational Institutions including Universities

Chang Jae Lee

Education Facility Disaster Association, Korea

Even though Korea has been considered as a safe nation towards earthquakes, recent earthquakes in the areas of Kyungjoo and Pohang have reminded us that severe earthquakes could be occurred in Korea in the future and there has been increasing anxiety among Koreans.

However, recent nationwide protective measures against earthquakes have focused on the structural safety of buildings and structures and most of the investments from the government has distributed to improve the design and reinforcement for earthquake-proof structures. Therefore, relatively little attention has been paid to the nonstructural factors that are responsible for the most secondary damages caused by earthquakes.

Explosive and inflammable high-pressure gas and chemicals stored in the laboratories of universities may cause severe damages against personnels in the institutions. Therefore, newly published guide will show basic protective methods from the hazard elements in the laboratories for the reduction of physical damages from earthquakes.

Symposium : **KCS6-2**
[Laboratory Safety Education] Laboratory Safety Education for the Graduate Students
Room 602, FRI 09:40
Chair: Ik-Mo Lee (Inha University)

Cognitive-Behavioral Approach to Safety

ChangHo Park

Department of Psychology, Chonbuk National University, Korea

Human errors are considered as serious threats to not only industrial but also laboratory safety. Lack of safety awareness is often blamed as one of major causes of human errors, so much effort has been given to enhance safety awareness. It is thought that understanding psychological mechanisms of human errors would contribute to changing our safety awareness and behavior deeply. Major psychological processes such as attention, memory, and thinking, often involved in human errors and accidents as well, are discussed. And several measures against human errors are suggested in relation to such processes. Next, principles of human learning is introduced which could be applied to safety behavior analysis and for behavioral change.

Symposium : **KCS6-3**
[Laboratory Safety Education] Laboratory Safety Education for the Graduate Students
Room 602, FRI 10:20
Chair: Ik-Mo Lee (Inha University)

Characteristics of Chemicals and Examples of Accidents

Ik-Mo Lee

Department of Chemistry, Inha University, Korea

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

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

Symposium : **POLY1-1**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 700A, THU 15:40
Chair: Hyung-il Lee (University of Ulsan)

Supramolecular Polymers from Functional Hydrazones: Helicity Control and Aggregation Induced Emission

Kyung-su Kim, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Stimuli-responsive or controlled self-assembly has been intensively investigated over the years for various applications such as bio-sensing, drug delivery, and actuators. Hydrazone functional groups have the advantage to be applied in such materials due to their dynamic property of the reversible C=N bond. In this talk, novel hydrazone derivatives were discussed, which show concentration-dependent equilibrium of a hydrazone and its dimer or aggregates. This phenomenon was also affected by protonation/deprotonation equilibria. The self-assembly of those hydrazones could be controlled not only by pH variation but also by dynamic covalent exchanges. In addition, the introduction of a chiral auxiliary group gave rise to the supramolecular chirality, which can be controlled by kinetic or thermodynamic conditions. Lastly, it was discovered that certain hydrazone derivatives showed aggregation-induced emission (AIE). Its origin will be discussed in terms of their molecular structures.

Symposium : **POLY1-2**

Special Symposium by Mid-career Polymer Synthesis Scientists

Room 700A, THU 16:10

Chair: Hyung-il Lee (University of Ulsan)

Synthesis and Application of Novel Polymer Networks having Covalent Polysulfide Linkages

Yong Seok Kim

Advanced Functional Polymers Research Center, Korea Research Institute of Chemical Technology, Korea

The synthesis and characterization of poly-(phenylene polysulfide) networks (PSNs) with controlledaverage sulfur ranks, from elemental sulfur (ES) and pdiiodobenzene (DIB), are investigated. The PSN films,prepared via simple hot pressing, are found to possess large extensibility up to around 300% and complete recovery of shape and mechanical properties after deformation, which are attributed to the loosely cross-linked network structures mainly consisting of linear poly(phenylene polysulfide) chains.The covalent polysulfide linkages in the PSNs also exhibit dynamic behaviors under ultraviolet (UV) or thermal treatment, thus, enabling self-healing and reprocessing of the films when scratched and broken, respectively. Combined with the unique mechanical properties of the PSNs, their high refractive index and excellent infrared (IR) transparency contribute to the preparation of stretchable, healable, and reprocessable IR transmitting materials for potential deformable and stretchable optical applications.

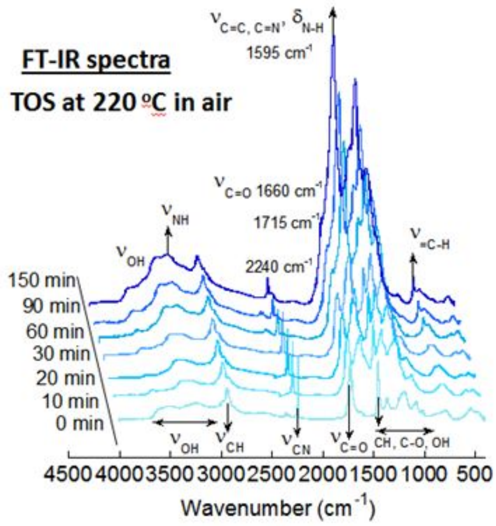
Symposium : **POLY1-3**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 700A, THU 16:40
Chair: Hyung-il Lee (University of Ulsan)

Efficient structural transformation of polyacrylonitrile copolymers during thermal oxidative stabilization for carbon materials

Sung Chul Hong

Department of Nanotechnology and Advanced Material, Sejong University, Korea

As one of the most important carbon precursors for manufacturing carbon materials, polyacrylonitrile (PAN) copolymers have attracted significant attention by both industry and academia. Thermal oxidative stabilization (TOS) is indispensable step for the formation of carbon materials from the PAN copolymer precursors. In this study, Fourier transform infrared spectroscopy (FT-IR) was employed for the quantitative tracking of the structural evolution of the PAN copolymers during TOS. The TOS process includes cyclization, oxidation and tautomerization, as characterized by the evolution of corresponding peaks in FT-IR. The preparations of model PAN copolymers were carefully designed to provide PAN copolymers with different comonomers, compositions and chain architectures. PAN copolymers containing approximately 3 mol% of itaconic acid exhibited efficient TOS process in terms of cyclization, oxygen uptake and dehydrogenation reactions. The PAN copolymers with block architectures, uniformly distributed comonomer along the chain, or high isotacticity also demonstrated improved TOS processes compared with that of random atactic PAN copolymers. The stabilization behaviors of PAN copolymers were also investigated under electron beam irradiation at room temperature to investigate the TOS mechanism. The carbon materials produced through the efficient TOS and carbonization of tailored PAN copolymers were promising materials for applications in the field of carbon technology. As an example of such applications, a core-shell structured hybrid nanofiber composed of carbonized PAN copolymer and Pt nanoparticles were prepared, exhibiting improved energy conversion efficiency in dye-sensitized solar cell as a counter electrode.


FT-IR spectra
TOS at 220 ºC in air
$\nu_{C=C,\ C=N}$, δ_{N-H}
1595 cm^{-1}
$\nu_{C=O}$ 1660 cm^{-1}
1715 cm^{-1}
2240 cm^{-1}
ν_{OH}
ν_{NH}
$\nu_{=C-H}$
150 min
90 min
60 min
30 min
20 min
10 min
0 min
ν_{OH}
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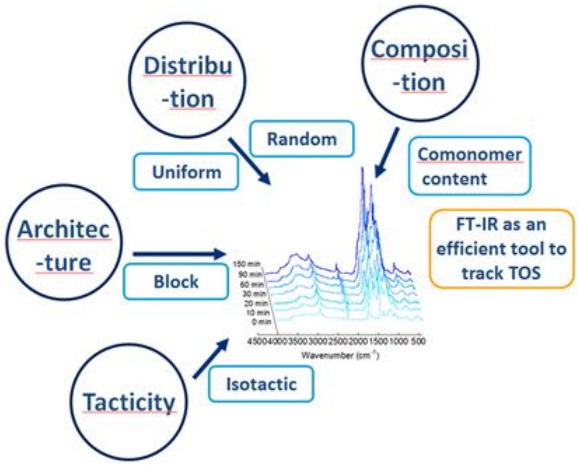
ν_{CN}
$\nu_{C=O}$
CH, C-O, OH
4500 4000 3500 3000 2500 2000 1500 1000 500
Wavenumber (cm^{-1})


Distribu-tion
Composi-tion
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Architec-ture
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FT-IR as an efficient tool to track TOS
Tacticity
Isotactic
150 min
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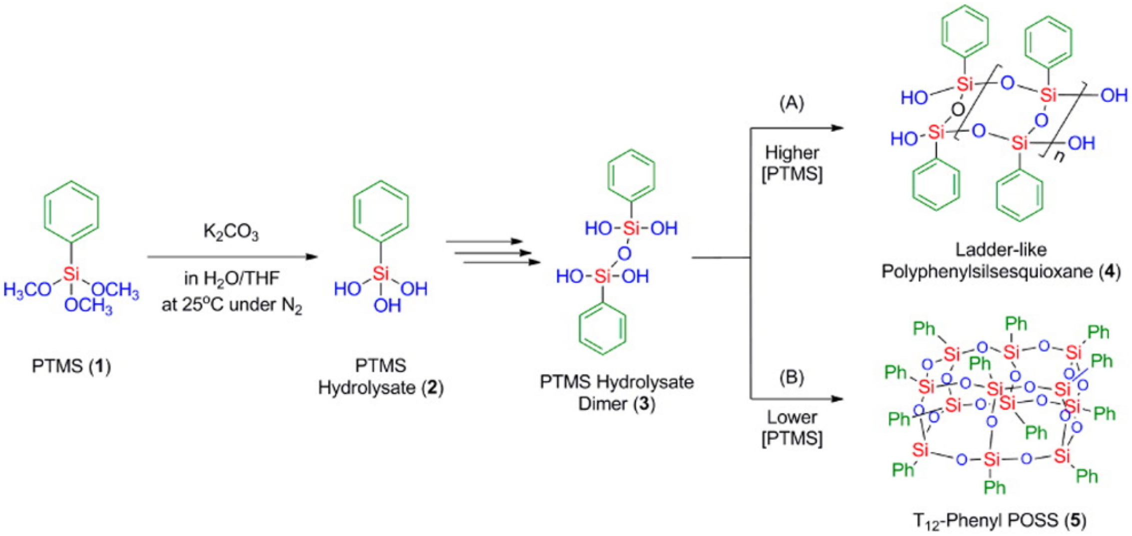
Symposium : **POLY1-4**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 700A, THU 17:10
Chair: Hyung-il Lee (University of Ulsan)

Synthesis of Structure Controlled Polysilsesquioxanes and its applications

Kyung-Youl Baek

Center for Materials Architecturing, Korea Institute of Science and Technology, Korea

Polysilsesquioxanes (PSQ) comprise of a class of inorganic-organic hybrid materials that exhibit unique physical and chemical properties unrealized in purely organic or inorganic sources. These materials have shown advantageous properties such as excellent thermal stability, low dielectric constant, good mechanical properties, chemical resistance, and even biocompatibility. Of the three known structural classes of PSQs: random branched sols, polyhedral oligomeric silsesquioxanes (POSS), and ladder-like polysilsesquioxanes (LPSQ), only POSS and LPSQ can be characterized to be of controlled structures, where POSS generally possess oligomeric three-dimensional cage structures while a hypothetical LPSQ is a polymeric analogue with linear, double-strained siloxane backbone. However, the synthesis for these controlled structures often required restricted and cumbersome reaction steps with experienced techniques, because of high reactivity of alkylsiloxane monomers. In this presentation, I will show the synthetic feasibility of these structure controlled poly(phenylsilsesquioxane) using a mild base catalyst systems at room temperature to give T12-Phenyl POSS or ladder-like poly(phenylsilsesquioxane) (LPPSQ) by control of initial phenyltrimethoxysilane (PTMS) concentration in excellent yields (Scheme 1). In addition, some applications will be shown in the fields required specific properties of PSQs.


H$_3$CO
Si
OCH$_3$
OCH$_3$
PTMS (**1**)
K$_2$CO$_3$
in H$_2$O/THF
at 25^{o}C under N$_2$
HO
Si
OH
OH
PTMS
Hydrolysate (**2**)
HO-Si-OH
O
HO-Si-OH
PTMS Hydrolysate
Dimer (**3**)
(A)
Higher
[PTMS]
(B)
Lower
[PTMS]
HO
Si
O
Si
OH
HO
Si
O
Si
OH
n
Ladder-like
Polyphenylsilsesquioxane (**4**)
Ph
Si
O
T$_{12}$-Phenyl POSS (**5**)

Symposium : **POLY2-1**

Recent Trends in Early-career Polymer Chemists

Room 606, FRI 09:00

Chair: Min Sang Kwon (UNIST)

Methodological approach on curing reaction of liquid crystalline epoxy resin for developing thermally conductive networks

Hyeonuk Yeo

Department of Chemistry Education, Kyungpook National University, Korea

My talks will be on our group’s recent works to develop liquid crystalline epoxy resins (LCERs) with high thermal conductivity. First, we synthesized a typical LCER bearing 4,4’-biphenyl mesogenic moieties and studied its curing reaction with various diamine hardeners. In the studies, well-aligned liquid crystalline networks were found to be disturbed during the curing process. Two reasons were considered: first, a large amount of non-liquid crystalline components were introduced as a curing agent capable of inhibiting the alignment of the liquid crystalline phase. Second, an amorphous network structure was highly developed during the crosslinking process occurred by the diamine hardeners. To solve the above problem, we developed a new type hardener which enabled catalytic polymerization of the LCER. As a result, the content of curing agent was greatly lowered, which obviously contributed to the improvement of crystallinity. It was possible to maximize the self-orientation of the LCER, which influenced the improvement of the thermal conductivity. In addition, using the same curing system, LCER composites with h-BN were fabricated. The composites showed remarkably high thermal conductivity as we intended. In the symposium, the details will be presented.

Symposium : **POLY2-2**
Recent Trends in Early-career Polymer Chemists
Room 606, FRI 09:25
Chair: Min Sang Kwon (UNIST)

Adaptive Supramolecular Nanomaterials

Yongju Kim

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

Molecular assembly forms diverse supramolecular architectures through non-covalent interactions which can be changed reversibly by external stimuli such as temperature, light, salt, and pH. I present the switchable assembly by adjusting non-covalent interactions for 1D tubules and 2D porous sheets. For example, dynamic tubular pores undergo rapid switching between open and closed states in response to a thermal signal in water. Notably, this pore switching mediates a controlled water-pumping catalytic action for the dehydration reaction. A virus-like hierarchical assembly with the native DNA and a synthetic coat shows repeated collective helicity switching triggered by pH change. This collective helicity inversion occurs during translocation of the DNA–coat assembly into intracellular compartments. Translating DNA conformational dynamics into a higher level of hierarchical dynamics may provide an approach to create DNA-based nanomachine. Homochiral porous nanosheets are presented with open-closed pore switching. The porous 2D structures can serve as enantiomer sieving membranes which exclusively capture a single enantiomer in a racemic mixture solution with high uptake capacity. The entrapped guests inside the pores can be pumped out by pore closing triggered by salt. Moreover, I also present supramolecular concepts to translate the adaptive nature of biological systems into synthetic self-assembly.

Symposium : **POLY2-3**
Recent Trends in Early-career Polymer Chemists
Room 606, FRI 09:50
Chair: Min Sang Kwon (UNIST)

Selective De-Cross-Linking Enables Macroscopic Responses in Double-Network Hydrogels

Hyungwoo Kim

School of polymer science and engineering, Chonnam National University, Korea

Since the concept for protection−deprotection reactions was discovered, the orthogonality has been remarkably developed, and now it not only suggests practical synthetic routes but also provides feasible pathways to realize complex chemical designs of diverse polymeric materials that are highly sought-after. The approach has been employed to synthesize sophisticated yet practical polymeric structures, and manipulate behavior of polymeric materials in parallel, which now enables amplifying signals, tuning large-scale properties of materials, or mimicking biological functions. In that sense, this presentation exhibits the design of macroscopic responses in thermosetting hydrogels via selective de-cross-linking. The selective de-cross-linking can be achieved simultaneously or continuously dependent on the designed structures of materials, and dramatically reverse macroscopic properties leading to controlled release or transformation in the hydrogels.

Symposium : **POLY2-4**
Recent Trends in Early-career Polymer Chemists
Room 606, FRI 10:15
Chair: Min Sang Kwon (UNIST)

Design of Stimuli-responsive Organic Molecules and Polymers based on the Controlled Intermolecular Interactions

Kyeongwoon Chung

Korea Institute of Materials Science (KIMS), Korea

Rational material design is critical to fully realize the properties of organic conjugated materials in applications, by regulating their intermolecular packing as well as intramolecular properties. Indeed, Investigation on molecular design principles can depict an insightful picture on how properties of conjugated organic molecules and polymers can be designed and fully utilized in various applications. In this talk, the molecular design strategies to control interactions and assemblies of organic conjugated materials will be discussed, which enables unique optical and electronic properties for various applications. First, a molecular design to control intermolecular interactions renders a unique thermally stable supercooled liquid and its shear-triggered lighting-up crystallization which enables highly sensitive crystallization of the supercooled liquid even by living cell attachment. Furthermore, based on controlled subtle interaction differences between substrate, fluorescent sensory molecules, and analyte solvents, a novel optical sensor is devised. The highly selective sensor array can clearly distinguish physicochemically similar liquids; ethanol, methanol, ethylene glycol, and water. Insightful design consideration for both intrachain and interchain properties is also critically important for conjugated polymers (CPs). A molecular design of CPs' main and side chains to regulate optical properties will be introduced. Based on the sophisticatedly tailored optical properties of CPs, latent optical information encoding using CPs as security inks is demonstrated, which reveals and conceals hidden information upon CP aggregation/deaggregation.

Symposium : **POLY3-1**

Recent Trends in Environmental Science-Related Polymer Research

Room 700A, FRI 14:30

Chair: Sung Cheol Yoon (KRICT)

Biobased and Biodegradable Plastics

Dongyeop Oh

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

China had been imported half of the wolrd plastic waste, including hunder thousands tons from Korea annually. Due to China’s new import policy, plastic wastes began piling up thoughout he mountains and fields of Korea. Another important issue is "chemophobia". Plastic contains hamful additives, preservatives and other chemicals. For example, bisphenols found in plastic food packaging and can linings is closely linked to endocrine disruption, nervous and immune disfunctions. Bio-based and/or biodegradable plastics have been being considered as the solution for both issues. This talk presents an overview of facts and recent (our) research progress in bio-based and/or biodegradable plastics.

Symposium : **POLY3-2**
Recent Trends in Environmental Science-Related Polymer Research
Room 700A, FRI 14:55
Chair: Sung Cheol Yoon (KRICT)

Nanopolysscharides and their applications

Dong Soo Hwang

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

Cellulose and chitin are two most abundant natural polymers present in nature (1010~12 ton/year). Both are sustainable and renewable biopolymers that are produced form various resources like bacteria, fungi, plant and animals. Most functional groups in both polymers are used to form naturally occurring nanofibers with high crystallinity with a diameter range from 2 to 20 nm. The nano-fibrous structure of cellulose and chitin has attracted public attention as a source for new advanced material because the nanofibers have not only superior mechanical properties (~50 GPa of stiffness) but also numerous chemical moieties which can be used for tuning chemical activities depending on a variety of the application fields. However, isolation of the nanofibrous structures from natural resources had been limited because both cellulose and chitin are neither meltable nor soluble in most commonly used solvents. Processes involving harsh chemical and ionic liquid treatments have been used to isolate the cellulose and chitin from the natural resources but it results in the destruction of the nano-crystalline structures of them. Recently, by introducing carboxyl groups into native cellulose or chitin through (2,2,6,6-tetramethylpiperidin-1-yl)hydroxyl (TEMPO) mediated oxidation and mechanical grinding, nanofibers with a uniform diameter were successfully obtained. Cellullose and chitin nanofibers from TEMPO/NaClO/NaBr system show exceptional mechanical properties and large surface area with low cost. In this presentation, current research trends and their application of the cellulose and chitin nanofibers will be presented.

Symposium : **POLY3-3**
Recent Trends in Environmental Science-Related Polymer Research
Room 700A, FRI 15:20
Chair: Sung Cheol Yoon (KRICT)

Microparticles efficiently remove copper ion, retain their structure in aqueous media, and eventually degrade after use

Jeyoung Park

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

Key-requirement for organic pollutant-adsorbent materials in aqueous media is the balance of efficiency and biodegradation due to emerging microplastic pollution issues. Hyperbranched polyamidoamine-based micro-hydrogel particles showed highly efficient absorbent for removing heavy metal ions, however, impatiently hydrolyzed before fully functioning in a polluted water. Herein, lysine-cyclomer is copolymerized with diamine and diacrylamide via an inverse suspension polymerization, thereby giving a high performance copper ion-absorbent materials with controlled degradation in aqueous media. This study suggests long-lasting absorbent for water-purification industries without environmental burden.

Symposium : **POLY3-4**
Recent Trends in Environmental Science-Related Polymer Research
Room 700A, FRI 15:45
Chair: Sung Cheol Yoon (KRICT)

Carbonization of silk protein into pseudographitic pyroprotein

Se Youn Cho

Carbon Convergence Materials Research Center, Korea Institute of Science and Technology, Korea

Silk proteins are of great interest to the scientific community owing to their unique mechanical properties and interesting biological functionality. In addition, the silk proteins are not burned out following heating, rather they are transformed into a carbonaceous solid, pyroprotein; several studies have identified potential carbon precursors for state-of-the-art technologies. However, no mechanism for the carbonization of proteins has yet been reported. Here we examine the structural and chemical changes of silk proteins systematically at temperatures above the onset of thermal degradation. We find that the sheet structure of the silk proteins is transformed into an sp2-hybridized carbon hexagonal structure by simple heating to 350 ℃. The pseudographitic crystalline layers grew to form highly ordered graphitic structures following further heating to 2,800 ℃. We provide a mechanism for the thermal transition of the protein and the graphitization behaviour. In addition, control over sheet structure of the silk proteins resulted in different carbon microstructures, and nanocarbons with one-, two- and three-dimensional morphologies were fabricated from the regenerated silk proteins. This demonstrates that it is possible to fabricate carbon materials with controlled microstructure and morphology via a wet process.

Award Lecture in Division : **INOR1-1**
Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry
Room 302, THU 15:40
Chair: Youngjo Kim (Chungbuk National University)

Pushing the Limits of N-heterocyclic Carbenes

Eunsung Lee

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

N-Heterocyclic Carbenes (NHCs) have been intensively explored for stabilizing unstable species such as radicals and zerovalent nonmetal species, and for activating small molecules such as CO, H2, NH3, N2O, NO, etc.[1,2] Such a capability of NHCs can be attributed to their strong donor characters and steric tunability that lead to the remarkable reactivity. Recently, we reported N-heterocyclic carbene nitric oxide (NHCNO) radicals, which can be also considered as iminoxyl radicals. NHCNO radicals react with silyl and alkyl triflate to generate the corresponding radical cations.[3] The structures of the unprecedented oxime ether radical cations were determined by X-ray crystallography. Furthermore, we also found that triazenyl cations stabilized by NHC form the corresponding triazenyl radicals upon the treatment of elemental potassium as a reductant.[4] The triazenyl radicals were fully characterized by single-crystal X-ray analysis and electron paramagnetic resonance (EPR) spectroscopy. The details of synthesis, characterization, and formation mechanisms of the compounds will be discussed. References:[1] J. Park, H. Song, Y. Kim, B. Eun, Y. Kim, D. Y. Bae, S. Park, Y. M. Rhee, W. J. Kim, K. Kim, E. Lee. J. Am. Chem. Soc. 2015, 137, 4642. [2] H. Song, Y. Kim, J. Park, K. Kim, E. Lee. Synlett. 2016, 27, 477. [3] Y. Kim, K. Kim, E. Lee. Angew. Chem. Int. Ed. 2018, 57, 262. [4] J. Back, J. Park, Y. Kim, H. Kang, Y. Kim, M. J. Park, K. Kim, E. Lee. J. Am. Chem. Soc. 2017, 139, 15300.

Award Lecture in Division : **INOR1-2**
Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry
Room 302, THU 16:05
Chair: Youngjo Kim (Chungbuk National University)

Zintl Phase Solid-State Compounds for Energy Material Applications

Tae-Soo You

Department of Chemistry, Chungbuk Natioanl University, Korea

The Zintl phase A5M2Pn6 (A = Ca, Sr, Eu, Yb; M = Al, Ga, In; Pn = As, Sb, Bi) series has been extensively investigated by worldwide researchers for thermoelectric applications. Our recent studies for the Ca5-xYbxAl2Sb6 ($1.0 \le x \le 5.0$) system, where two cations of Ca and Yb formed a solid-solution mixture, revealed that some Yb-rich compounds with a particular range of composition originally adopted the Ba5Al2Bi6-type phase, but they underwent a structural transformation to the Ca5Ga2As6-type phase during the post-heat-treatment. Moreover, their conductivities were also shifted from metallic to semiconducting during this phase transition. After then, we attempted to apply an anionic p-type dopant Ge in the Ca5-xYbxAl2Sb5-xGey system and successfully enhanced the Seebeck coefficient. In addition, we also proved that originality of the structural transformation was descended from the site-preference of Ca and Yb. To further expand our understanding about the A5M2Pn6 series, we applied the cationic n-type dopants using rare-earth metals (RE) and resulted in producing the quinary Ca5-x-yYbxREyAl2Sb6 (RE = Pr, Nd, Sm, Eu, Gd system. As RE3+ dopants were introduced in the Ca-rich compounds, the Ba5Al2Bi6-type phase initially crystallized, but after the post-heat-treatment, the original phase was successfully transformed into the Ca5Ga2Sb6-type phase. Quite interestingly, along with this structural transition, we also observed the p-type to n-type conversion in the title compounds. To the best of our knowledge, this is the first example that shows the p-type to n-type conversion in the A5M2Pn6 (A = Ca, Sr, Eu, Yb; M = Al, Ga, In; Pn = As, Sb, Bi) series induced by the structural transformation from its original Ba5Al2Bi6-type to the Ca5Ga2As6-type phase. To understand this kind of intriguing p-type to the n-type conversion along with its related TE properties, a series of theoretical DFT calculations using several hypothetical models were also performed, and the resultant DOS, COHP, ELF and band structure were thoroughly analyzed.[References]1. Nam, G.; Choi, W.; Jo, H.; Ok, K.; Ahn, K. and You, T.-S. Chem. Mater. 2017, 29, 1384-1395.2. Lim, S.; Nam, G.; Shin, S.; Ahn, K.; Lee, Y. and You, T.-S. Inorg. Chem. 2019, 58, 5827-5836.

Symposium : **INOR1-3**

Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry

Room 302, THU 16:30

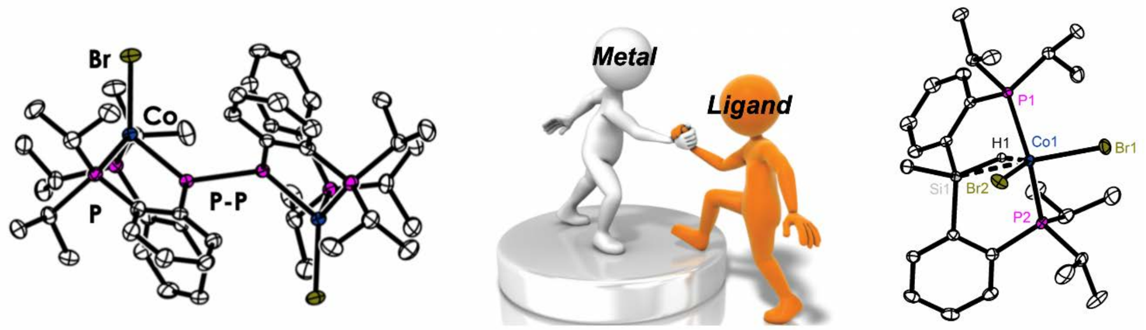
Chair: Seungwoo Hong (Sookmyung Women's University)

Metal-Ligand Cooperative Transformation of Small Molecules Inspired by Metalloenzyme Reactions

Yunho Lee

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

Transition metal mediated transformations of small molecules such as N2, H2, COx and NOx are drawing much attention due to their importance in understanding various metalloenzyme reactions. Several enzymes utilize the cooperativity between a metal ion and amino acid residues in their active site for processing biologically important chemical transformations. Inspired by such cooperative reactions, we employ metal-ligand cooperation (MLC) as a novel synthetic methodology to expand the role of transition metals in small molecule conversion. While non-innocent phosphide and silyl ligands are relatively rare, our group recently reported a new type of metal-ligand cooperation by using an anionic PEP ligand (E = P or Si). In a PPP system, the central phosphide moiety can be a 1 or 2 electron donor, which was recognized from the studies of various nickel and cobalt complexes. In this presentation, the MLC redox chemistry of a (PPP)M scaffold (M = Ni or Co) and its application in C1 conversion will be presented. Both nickel and cobalt complexes reveal the reversible formation of a P–P bond involving a single electron exchange between metal and P. By using this reversible conversion, a synthetic cycle for isocyanate generation starting from the nickel amide species was successfully accomplished. Various bond activations are achieved at the M-P-P-M site, which is equivalent to the metal-phosphinyl radical operating as an active MLC site. Secondly, the unusual Si–M cooperative reactions of the divalent nickel complexes supported by an anionic PhSiP2 ligand will be presented. Coupled with a redox change of a metal ion, the cooperativity of the silyl metal moiety was established with a series of experimental and theoretical evaluations.


Br
Co
P
P-P
Metal
Ligand
P1
H1
Co1
Br1
Si1
Br2
P2

Symposium : **INOR1-4**
Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry
Room 302, THU 16:50
Chair: Seungwoo Hong (Sookmyung Women's University)

Artificial Cell Signaling by Using a Cobalt(III)-Nitrosyl Complex with Light

Jaeheung Cho

Emerging Materials Science, DGIST, Korea

Cells use enzymatically synthesized gaseous molecules such as nitric oxide (NO) to transmit both of intracellular and intercellular signals. In principle, the endogenous small molecules precisely regulate physiological changes, but it is unclear how randomly diffusive molecules trigger and discriminate signaling programs. Here, we show that gasotransmitters use time-dependent dynamics to discriminate the endogenous and exogenous inputs. For a real-time stimulation of cell signaling in live cell, we synthesized a chemical delivery tool a photo-cleavable metal-nitrosyl complex, [CoIII(MDAP)(NO)(CH3CN)]2+ (MDAP = N,N'-dimethyl-2,11-diaza[3,3](2,6)pyridinophane), which can stably deliver and selectively release NO with fine temporal resolution in the cytosolic region. It has been characterized by crystallographic and spectroscopic methods and it releases NO with a high quantum efficiency (ΦNO = 0.78) in H2O, upon activation with light. Theoretical calculations support our interpretation that the dissociation of NO occurred in the singlet excited state. We demonstrate its utility by investigating the extracellular signal–regulated kinases (ERKs). By measuring the dynamics of ERK responses using a kinase translocation reporter (KTR) in a live cell, we revealed how the cells use both exogenous and endogenous NO to disentangle cellular responses. This activation technique can be used not only to understand how diverse cellular signaling networks are interconnected dynamically but also to control drug delivery system precisely.

Symposium : **INOR1-5**
Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry
Room 302, THU 17:10
Chair: Seungwoo Hong (Sookmyung Women's University)

Metal Complexes for Visualization and Photocontrol of Biological Zinc

Youngmin You

Division of Chemical Advanced Materials, Ewha Womans University, Korea

Biological zinc plays key roles in a variety of the physiological processes, including synaptic transmission. Growing evidence also indicates that failures in the regulation of biological zinc are intimately linked to serious pathological conditions. However, chemical mechanisms underlying the zinc-mediated pathophysiology remains elusive, which attributes to the lack of proper probes. Photoluminescence, molecular probes are the most promising in the study of biological zinc with respect to non-invasiveness and spatiotemporal resolutions of zinc imaging. Our group has focused on the development of phosphorescence probes of judiciously tuned zinc binding ability. Molecular platforms of the probes were based on cyclometalated Ir(III) complexes, as they exhibit high-efficiency room temperature phosphorescence. The probes enabled time-resolved and lifetime-based photoluminescence detection of mobile zinc in the pools of mammalian cells and hippocampal slices. Our continued biological experiments further revealed the phototherapeutic actions of the phosphorescence probes due to sensitization of highly reactive oxygen species in the biological milieu. Taking advantage of these properties, photoactivatable prodrugs were synthesized and evaluated. Our research demonstrates promising utility of the complexes of late transition metals, including Ir(III), for study of the chemistry of bioinorganic species.

Symposium : **INOR1-6**
Recent Trends in Inorganic Chemistry I: Bioinorganic Chemistry
Room 302, THU 17:30
Chair: Seungwoo Hong (Sookmyung Women's University)

Electrocatalytic H2 Evolution Systems Inspired by Hydrogenases Active Sites

Junhyeok Seo

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

Hydrogenases are metalloenzymes that involve energy metabolism in microbial communities as catalyzing the reversible oxidation of molecular hydrogen. The enzyme family is classified into three kinds, [FeFe]-, [NiFe]-, and [Fe]-hydrogenase. The dinuclear [FeFe], [NiFe]-hydrogenases have been studied in detail about their redox activity in the H2 generation and metabolism. The [FeFe]-hydrogenase active site is composed of a diiron coordination center along with two functional sites of the electron-transfer and the proton delivery in the secondary coordination sphere. We synthesize molecular electro-catalysts inspired by the enzyme active site structure. A pincer type complex is used to link a conduit unit and a proton-relay functional group. I will present the synthetic strategy of the current H2 evolution catalysts and discuss the different reactivity depending on the metal center identity, the ligand functional group, and the complex geometry. In an extended research interest of the photon/electric energy conversion to a chemical binding energy of H2, we try to conjugate the H2 evolution catalyst to a water oxidation (photo)anode material. We utilize metal oxides composites to develop (photo)anode materials for the PEC water oxidation. In the seminar, I will discuss current efforts to develop the (photo)electrocatalysts for the H2 generation and water oxidation.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Symposium : **INOR2-1**

Recent Trends in Inorganic Chemistry II: Organometallic and Inorganic Materials Chemistry

Room 302, FRI 09:00

Chair: Bo Keun Park (KRICT)

Development of Formamidinium Tin Halide Perovskite Thin Film for Photovoltaic Applications

Seon Joo Lee

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

Inorganic-organic lead halide perovskite has been regarded as a promising light-absorbing material in photovoltaics because of its excellent optical, electrical properties and easy thin film fabrication. Recently, the power conversion efficiency (PCE) of lead-based perovskite solar cells (PSCs) has achieved more than 25%. However, the toxicity issue for lead (Pb) has been constantly addressed and it limits the further practical commercialization of lead-based PSCs. In this regard, many researchers have studied about the perovskite absorbing layers including Sn, Bi, Ge, and Sb as an alternatives to Pb, over the last five years. Among them, only tin(Sn)-based perovskite materials have produced an encouraging device performance up to now. However, the instability of Sn^{2+} upon exposure to air is still a bottleneck which causes the unwanted p-type doping in the perovskite film. In this presentation, I will give a brief review on the recent progress of tin-based PSCs and introduce the fabrication of formamidinium tin halide perovskite thin film and our approaches to reduce Sn vacancy caused by the oxidation of Sn^{2+}.

Symposium : **INOR2-2**

Recent Trends in Inorganic Chemistry II: Organometallic and Inorganic Materials Chemistry

Room 302, FRI 09:20

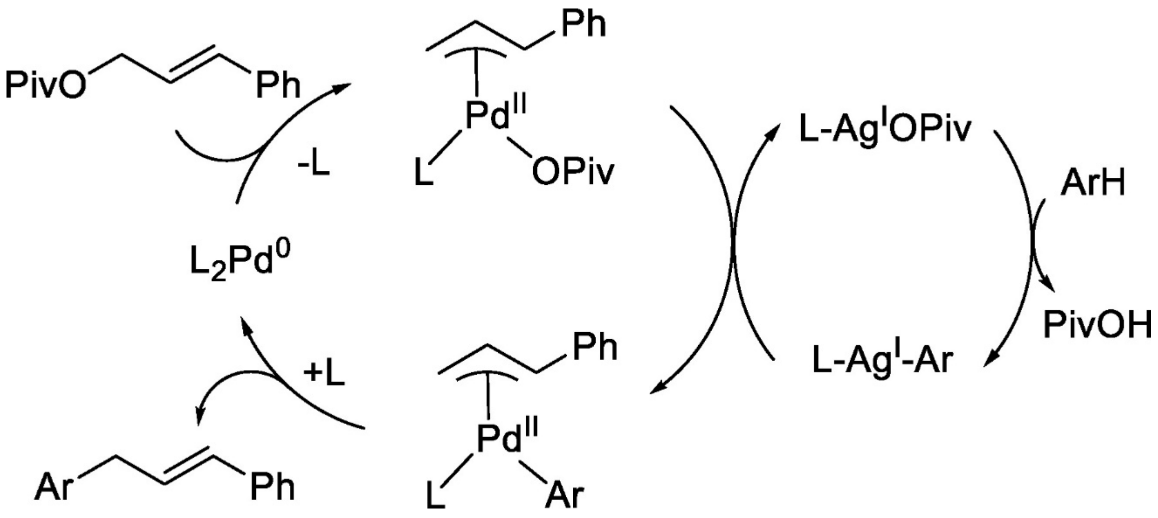
Chair: Bo Keun Park (KRICT)

Mechanistic Studies of Palladium-Catalyzed, Site-Selective Direct Allylation of Arenes by Silver-MediatedC–H Activation

Sarah Yunmi Lee, John F. Hartwig[1,*]

Department of Chemistry, Yonsei University, Korea
[1]*Department of Chemistry, University of California, Berkeley, United States*

Development and mechanistic investigations on a palladium-catalyzed direct allylation of arenes by silver-mediated C-H bond cleavage will be presented. This process allows for the highly site-selective construction of C(aryl)-C(sp^3) bond by the reaction between simple arenes and allylic pivalates. Our mechanistic data indicates that AgOPiv ligated by a phosphine reacts with the arene to form an arylsilver(I) species, presumably through a concerted metalation-deprotonation pathway. The activated aryl group is then transferred to an allylpallaidum(II) intermediate afforded by oxidative addition of the allylic pivalate to the Pd(0) complex. Subsequent carbon-carbon bond-forming reductive elimination furnishes the allylation product and the Pd(0) species. The proposed intermediates, including an arylsilver complex, have been isolated, structurally characterized, and determined to be chemically and kinetically competent to be intermediates by the suggested elementary steps of the catalytic cycle.


PivO
Ph
Ph
Pd^{II}
L
OPiv
-L
L$_2$Pd^0
L-Ag^{I}OPiv
ArH
PivOH
L-Ag^I-Ar
+L
Ph
Pd^{II}
L
Ar
Ar
Ph

Symposium : **INOR2-3**

Recent Trends in Inorganic Chemistry II: Organometallic and Inorganic Materials Chemistry

Room 302, FRI 09:40

Chair: Bo Keun Park (KRICT)

Improved catalyst performance by SnOx overcoating using powder atomic layer deposition

Jeong Hwan Han

Seoul National University of Science & Technology, Korea

Tin based thin films (SnOx, SnSx) have attracted great attention due to its excellent electric and optical properties for the applications of complementary metal oxide semiconductor, photo and electrochemical catalysts, photovoltaic device, gas sensor and so on. Meanwhile, among various deposition techniques, atomic layer deposition (ALD) has been spotlighted due to its promising deposition features such as precise atomic level thickness/composition control and excellent coverage on the 3D structure substrates. In this presentation, we will introduce the phase-controlled growth of ALD SnOx films using newly developed metal-organic Sn precursor. Additionally, our recent achievements on the successful SnOx overcoating on various catalyst materials by fluidizing type powder ALD technique, and improved activity and stability of SnOx coated catalyst will be presented.

Symposium : **INOR2-4**
Recent Trends in Inorganic Chemistry II: Organometallic and Inorganic Materials Chemistry
Room 302, FRI 10:00
Chair: Bo Keun Park (KRICT)

Synthesis of Shape-controlled β-PdH Nanocatalysts for the Liquid Fuel Oxidation Reactions

Mrinal Kanti Kabiraz, Jeonghyeon Kim, Sang-Il Choi[1,*]

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

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

Symposium : **INOR2-5**
Recent Trends in Inorganic Chemistry II: Organometallic and Inorganic Materials Chemistry
Room 302, FRI 10:20
Chair: Bo Keun Park (KRICT)

Methane Oxidation to Methanol Precursor using Homogeneous Catalyst in Acid Media

Hyunjoo Lee

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

Catalytic activation of methane to valuable chemical such as methanol is an important issue from both a practical and academic standpoint. Due to its abundance and innocuous property, molecular oxygen-mediated direct oxidation of methane to methanol using a heterogeneous catalyst has been studied extensively. However, a high reaction temperature and the trade-off between conversion and selectivity limit this method due to the thermochemically stable methane and relatively less stable product, methanol. One way to overcome this dilemma is to oxidize methane to a methanol intermediate such as methyl bisulfate (CH_3OSO_3H). In this presentation, we review the recent catalyst development trends at the liquid-phase methane oxidation performed in acid media. We also show our results on oleum (SO_3-H_2SO_4)-mediated methane oxidation using organometallic platinum catalyst, $(DMSO)_2PtCl_2$, which has a higher activity and stability compared to previously reported Periana catalyst and K_2PtCl_4. The catalyst deactivation, reactivation and reaction mechanism will also be presented.

Symposium : **INOR3-1**

Recent Trends in Inorganic Chemistry III: Metal−Organic Frameworks

Room 302, FRI 14:30

Chair: Hyun Sung Kim (Pukyong National University)

Controlled manipulation of the porosity and rigidity characteristics of some zeolitic imidazolate frameworks

Jisu Lee, Kyungkyou Noh[1], Jaheon Kim[*]

Department of Chemistry, Soongsil University, Korea
[1]*Department of ICMC convergence technology, Soongsil University, Korea*

ZIFs are composed of divalent metal ions and imidazolate bridging ligand and tend to adopt zeolite-like structures. Unlike MOFs, there is no general strategy for targeting specific structures thus far, but it seems that functional groups in imidazole rings can affect significantly the stability of final structures based on limited examples. In spite of this difficulty in precise control of the ZIF structures, we have found several synthetic routes to functional ZIFs. First, we used metastable ACO and AFI ZIFs respectively to produce mixed-imidazolate ZIFs through reactions with extrinsic imidazoles. The introduction of the added imidazoles can lead to a change in framework topology and isoreticular products. Second, two SOD conformers could be synthesized separately under different solvent conditions. They show subtle but clear differences in the gas adsorption characteristics and can release gradually trapped benzene molecules upon heating under ambient atmosphere. This result implies that solvent molecules can act as a template for new ZIFs. Third, the rigidity of the ZIF framework can be controlled to give increased surface areas if the framework compositions are varied. For example, imidazole with small functional groups can be inserted into a rigid SOD framework, and bulkier imidazoles can make a flexible MER framework more rigid and more porous. Indeed, the increased surface areas are related to increased methane adsorption, which was confirmed by high-pressure measurements at room temperature. Similar to MOFs, all these examples indicate that the porosity and framework properties of various ZIFs can be modified in a controllable manner, which is advantageous for various applications such as gas storage and separation.

Symposium : **INOR3-2**

Recent Trends in Inorganic Chemistry III: Metal‒Organic Frameworks

Room 302, FRI 14:50

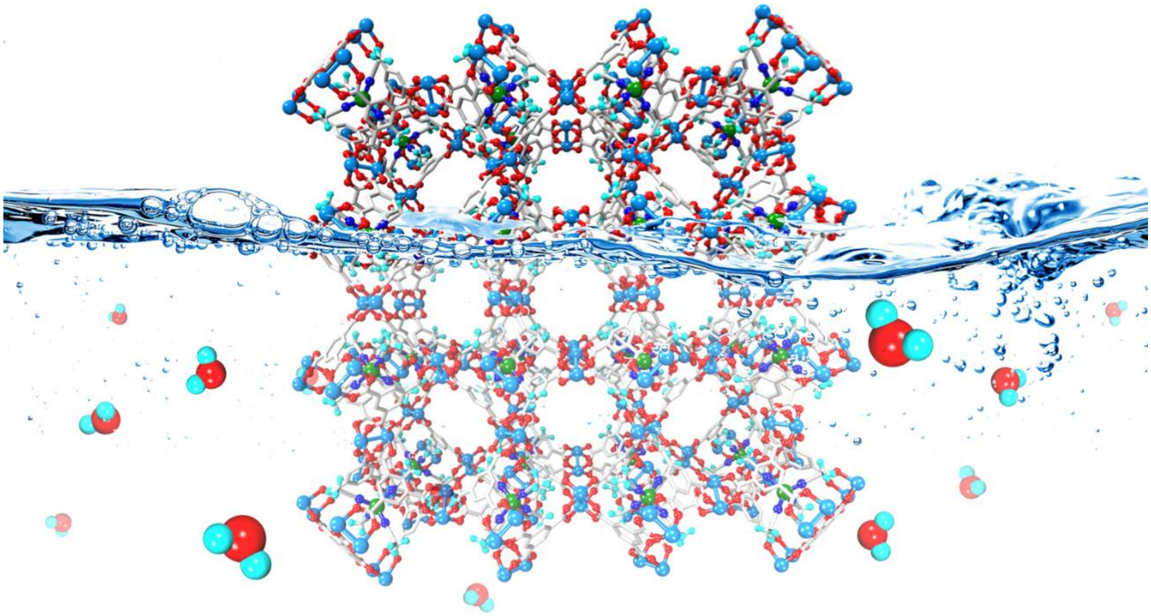
Chair: Hyun Sung Kim (Pukyong National University)

Coordinative Reduction: A Chemical Strategy to Enhance the Hydrolytic Stability of a Paddle-Wheel MOF

Nak Cheon Jeong

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

Enhancement of hydrolytic stability of metal‒organic frameworks (MOFs) is a challenging issue in MOF chemistry due to the limitation of their applications under a humid environment. Meanwhile, inner sphere electron transfer has constituted one of the most extensively studied subjects in contemporary chemistry. In this presentation, we show a new conceptual “coordinative reduction” of Cu^{2+} ion, which is realized in a paddlewheel MOF, HKUST-1, with a postsynthetic manner via inner sphere “single” electron transfer from hydroquinone (H_2Q) to Cu^{2+} through its coordination bond. H_2Q treatment of HKUST-1 under anhydrous conditions leads to the single charge (1+) reduction of approximately 30% of Cu^{2+} ions. Thus, this coordinative reduction is an excellent reduction process to be self-controlled in both oxidation state and quantity. More concretely, once Cu^{2+} ions are reduced to Cu^{+}, the reduction reaction does not proceed further, in terms of their oxidation state as well as their amount. Also, we show that a half of the Cu^{+} ions (about 15%) remains in paddlewheel framework with pseudo square planar geometry and the other half of the Cu^{+} ions (about 15%) forms $[Cu(MeCN)_4]^{+}$ complex in a small cage in the fashion of a ship-in-a-bottle after dissociation from the framework. Furthermore, we show that the coordinative reduction results in substantial enhancement of the hydrolytic stability of HKUST-1 to the extent that its structure remains intact even after exposure to humid air for two years.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **INOR3-3**

Recent Trends in Inorganic Chemistry III: Metal−Organic Frameworks

Room 302, FRI 15:10

Chair: Hyun Sung Kim (Pukyong National University)

Polymer@MOF Composites: Synthesis and Applications

Won Cheol Yoo

Department of Chemical and Molecular Engineering, Hanyang University, Korea

Metal-organic frameworks (MOFs) are well-known porous crystalline materials with high surface area and flexible structural and compositional tunabilities, which making them fascinating materials for applications in adsorption and separation. There are some drawbacks, however, such as chemical and physical instability, which become impeded versatile utilization of MOFs. Herein, I will present a facile strategy to improve moisture resistance of MOF by protecting metal sites with polymer. A site-specific polymerization that occurs at open metal sites of MOFs (Polymer@MOF) could be tunable through controlling degree of polymerization, resulting in controlled porosity of such composites. Improved stability of Polymer@MOF towards water compared to the pristine MOF (HKUST-1) will be introduced with consecutive water treatments and other possible applications of Polymer@MOF system will also be presented.

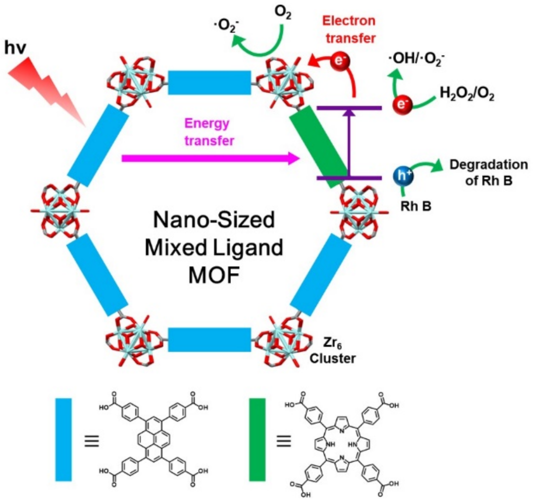
Symposium : **INOR3-4**
Recent Trends in Inorganic Chemistry III: Metal−Organic Frameworks
Room 302, FRI 15:30
Chair: Hyun Sung Kim (Pukyong National University)

Utilization of excited electron and energy in MOF-based photosensitizers.

Chang Yeon Lee

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

Well-arranged light-harvesting systems with complementary absorption and energy transfer processes between chromophores are indispensable in achieving successful imitation of natural photosynthetic systems. Metal−organic frameworks (MOFs), consisting of multi-dentate organic building blocks and metal or metal-cluster secondary building units, can be utilized as a photosensitizer to mimic photosynthetic systems due to their high regularity, superior synthetic versatility, and tailorable functionality. Since organic photosensitizers can be positioned periodically by coordination bond in the MOFs, it is possible to avoid their aggregation and self-quenching. Therefore, MOFs, possessing appropriate chromophores, has been employed as a new photosensitizer in various application fields such as photodynamic therapy (PDT) and photocatalysis. In this work, Zr-based nano-sized MOFs was decorated with a complementary chromophore (pyrene, porphyrin, and BODIPY) via mixed-ligands approach and solvent assisted ligand incorporation (SALI) method. Modified MOFs exhibit a significant improvement of reactive oxygen generation due to their enhanced light-harvesting properties.*This research was supported by the National Research Foundation of Korea funded by the Ministry of Science and ICT (NRF-2019R1F1A1059088).


hν
·O_2^-
O_2
Electron transfer
e^-
·OH/·O_2^-
e^-
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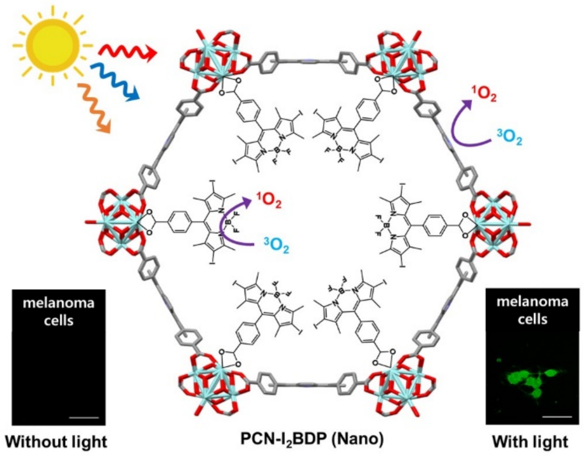
$^1O_2$
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melanoma cells
Without light
PCN-I_2BDP (Nano)
melanoma cells
With light

Symposium : **INOR3-5**
Recent Trends in Inorganic Chemistry III: Metal−Organic Frameworks
Room 302, FRI 15:50
Chair: Hyun Sung Kim (Pukyong National University)

Microporous Metal-Formate Frameworks: Unusual Proton Conduction Behavior and Gas Sorption Properties

Minyoung Yoon

Department of Chemistry, Kyungpook National University, Korea

Among various metal-organic frameworks, the framework comprising the smallest ligand, formate (HCO_2^-), cannot draw the attention of the researchers because of their poor porosity. Most of the metal-formate frameworks have been used for the study of magnetic property because of a magnetic couple of metal ions with short metal-metal distance. In 2004, Kim and coworkers reported one of the first porous metal-formate [α-$Mn(HCO_2)_2$] with gas sorption property.[1] Following the result, the selective gas sorption property of α-$M(HCO_2)_2$, where M = Mn, Mg, Co, and Ni, has studied. However, some of the unusual gas sorption properties cannot be explained only by the pore size of the framework. In addition, the very narrow 1-D channel may give interesting ion conduction behavior in high humidity conditions. Herein, we present the in-situ gas sorption structure analysis of α-$M(HCO_2)_2$ for the study of the unusual gas sorption selectivity of α-$M(HCO_2)_2$. Furthermore, the ion conduction behavior under high humidity conditions was investigated. Interestingly, the α-$M(HCO_2)_2$ structure was changed to the hydrated structure resulting in the superionic conduction. Furthermore, the framework showed the reversible crystal to amorphous phase change by changing the relative humidity. The unusual sorption and transport behavior of the metal formats can provide a new challenge in the application of the microporous metal-organic frameworks.[1] Dybtsev, D. N.; Chun, H.; Yoon, S. H.; Kim, D.; Kim, K. *J. Am. Chem. Soc.* **2004**, *126*, 32–33.

Symposium : **PHYS1-1**

Physical Chemistry Approaches in Advanced Materials

Room 600B, THU 15:40

Chair: Sangwoon Yoon (Chung-Ang University)

Optical properties of heterostructure nanorod laser

Jae Kyu Song

Department of Chemistry, Kyung Hee University, Korea

The optical properties of nanorods have not been well elucidated compared to macroscopic cavities, despite potential for photonic applications. Since the light-matter interaction are enhanced, the electromagnetic wave in nanorods is different from that in vacuum and bulk medium, which leads the formation of exciton-polariton to deviate from the classical electromagnetic wave theory. The optical properties of single nanolasers are investigated in InGaN/GaN heterostructure nanorods. Lasing occurs in the nanorods at low thresholds with high quality factors under ambient conditions. The spectral shift and spacing of Fabry-Perot-type modes imply a strong light-matter interaction in the reduced mode volume of the nanorods, which is explained by the exciton-polariton model. The polarization of the electric field in the lasing nanorods is perpendicular to the long axis of the nanowire and parallel to the substrate plane, which indicates that the Fabry-Perot modes belong to the same fundamental transverse mode. The dispersion curve of exciton−polariton model suggests that the group refractive index of polariton is significantly enhanced.

Symposium : **PHYS1-2**

Physical Chemistry Approaches in Advanced Materials

Room 600B, THU 16:10

Chair: Sangwoon Yoon (Chung-Ang University)

Atomic-Scale Understanding Microstructure-Property Relationships of Advanced Materials Using Electron Microscopy

Gyeong-Su Park

Materials Science & Engineering, Seoul National University, Korea

Recent progress in deliberate design and quality control of advanced emerging materials has opened a new exciting research area with the goal of extending their properties and performance that is increasingly linked to the specific microstructural phenomena. For this research, new analysis methods to identify the microstructure-property relationship are essential and it has recently been made possible thanks to the resolution and sensitivity available with the advent of high-performance electron microscopes. State-of-the-art electron microscopy achieved by the spherical aberration correction and the extremely narrow energy spread of electron beam not only provides structural and chemical information about the emerging materials even down to atomic resolution, but also enables to measure their dielectric properties (e.g., band gap, localized surface plasmon resonances). In addition, in-situ approaches to transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM) are able to provide dynamic information on the microstructure changes taking place in the materials exposed to some form of stimuli. These dynamic approaches to the electron microscopy can provide atomic level insights into materials functionality. This talk will present our latest research findings identified by a variety of TEM/STEM techniques on the correlation between microstructure and materials properties of semiconductor materials, energy materials, optical materials and bio-nanomaterials. In addition, this presentation will briefly introduce the TEM/STEM techniques applied to this study, including 3D electron tomography, monochromated electron energy-loss spectroscopy (EELS), and in-situ electrical probing inside TEM.

Symposium : **PHYS1-3**
Physical Chemistry Approaches in Advanced Materials
Room 600B, THU 16:40
Chair: Sangwoon Yoon (Chung-Ang University)

Optical Second-Harmonic Generation and its Interference in Atom-Thick Crystals

Sunmin Ryu

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

Atom-thick two-dimensional (2D) transition metal dichalcogenides (TMDs) with strong excitonic transitions in the NIR and visible range are excellent media for optical second-harmonic generation (SHG). SHG is not only a powerful structural method owing to its sensitivity to crystallographic symmetry, but also a coherent probe because of its instantaneous but non-dissipative response. In this talk,[1] I will present our recent findings on SHG interference occurring in 2D TMD heterostructures. All 2D crystal samples were prepared by mechanical exfoliation and characterized with a polarized SHG micro-spectroscopy setup powered by a tunable femtosecond Ti-sapphire laser. Polarization-resolved SHG polar plots of MoS2 homo-bilayers exhibited a six-petal pattern with six angular nodes like those of MoS2 monolayers. Remarkably, the SHG behavior of MoS2/WS2 was much different from that of MoS2 bilayers in that the former lacked angular nodes. This anomalous angular background became larger for more staggered hetero-bilayers, but decreased for increased fundamental wavelength. All the results were nicely explained by an SHG interference model considering material-dependent phase delay in their nonlinear response, which was corroborated with phase-resolved interferometric SHG measurements. I will also speak about our efforts on application of SHG spectroscopy in characterizing physicochemical changes in 2D crystals.[2,3]*******Reference*******[1] W. Kim and S. Ryu,* “Optical Second-Harmonic Interference in Atom-Thick Crystals”, To be submitted[2] Y. Ryu, W. Kim, S. Koo, H. Kang, K. Watanabe, T. Taniguchi, and S. Ryu,* “Interface-Confined Doubly Anisotropic Oxidation of Two-Dimensional MoS2”, Nano Lett. 17, 7267 (2017)[2] T. Y. Ko, A. Jeong, W. Kim, J. Lee, Y. Kim, J. E. Lee, G. H. Ryu, K. Park, D. Kim, Z. Lee, M. H. Lee, C. Lee and S. Ryu,* “On-Stack Two-Dimensional Conversion of MoS2 into MoO3”, 2D Materials 4, 014003 (2017)

Symposium : **PHYS1-4**

Physical Chemistry Approaches in Advanced Materials

Room 600B, THU 17:10

Chair: Hyuksang Kwon (KRISS)

Efficient and stable perovskite solar cells

Jangwon Seo

Korea Research Institute of Chemical Technology, Korea

Current perovskite solar cells (PSCs) intended for commercialization in the near future require both high efficiency and good long-term stability. Most highly efficient PSCs utilize an n-type layer of mesoporous titanium dioxide in an n-i-p device configuration, in which organic conductors are widely used to transport holes into an adjoined metal. Thus far, a variety of efforts have been devoted to achieve a defect-less perovskite film with high-quality morphologies to realize reduced loss-in-potential outcomes and enhanced efficiency levels. In this talk, we will discuss several challenges that need to be addressed in improving the photovoltaic performance and the stability of the perovskite solar cells, i.e. (1) preparation of high crystalline film of $(FAPbI3)_{1-x}(MAPbBr3)_x$ with a large grain size and a preferred orientation, (2) development of selective charge-transporting layers (CTL) with a superior stability, (3) interfacial control and energy level matching between the perovskite and the CTLs. We also continue to present our approach for realizing a long-term operating stability of PSCs with respect to the ion migration and the solid encapsulation. Our strategy as presented in this work will offer new directions for those involved in the fabrication of highly efficient and stable PSCs

Symposium : **PHYS1-5**
Physical Chemistry Approaches in Advanced Materials
Room 600B, THU 17:35
Chair: Hyuksang Kwon (KRISS)

Electrocatalyst for durable CO2 reduction reaction

Yun Jeong Hwang

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

Electrochemical CO2 reduction coupled with water splitting can provide a sustainable carbon cycle by combining with a renewable energy sources. In the fundamental level, many studies have been reproted to understand the electrocatalytic activity as well as the reaction pathways. Especially, the electrocatalyst design has been heavily focused on increasing the product selectivity and decreasing the overpotential at the initial state, which thus increase the energy efficiency of the electrolysis. However, long-term durability is also one of the important cirteria for practial application. The previous studies have been pointed out the morphology changes, deposition of the impurity or side products could cause fast deactivation of the electrocatalysts. Here, we are studying the advanced materials for high durability especially under the low-impurity electrolyte condition.

Symposium : **PHYS2-1**
Recent Progresses in Physical Chemistry
Room 600B, FRI 09:00
Chair: Kiyoung Park (KAIST)

Toward Higher Resolution in NMR Spectroscopy

Jung Ho Lee

Department of Chemistry, Seoul National University, Korea

Most nuclear spins in a molecule can generate nuclear magnetic resonance (NMR) signals. NMR spectroscopy becomes an atomic-resolution technique once we are able to resolve those signals. Routine application of Fourier-transform NMR, multidimensional approach, isotope enrichment, and high-field magnetic field separates most NMR signals from each other emanating from biomolecules. Intrinsically disordered proteins (IDPs) are abundant in the eukaryotic proteasome and are closely related to the pathogenesis of many degenerative disorders. Although NMR provides a unique way to investigate the atomic details of IDPs in solution, IDP NMR signals tend to substantially overlap, even with the application of above mentioned approaches.We developed a homonuclear decoupling method that narrows the amide-proton linewidths down to 3–5 Hz, without any of the artifacts observed in other homonuclear decoupling methods. The method employs a unique strategy to decouple the 3J couplings between alpha protons (HA) and amide protons (HN) by harnessing the seemingly unrelated 1J couplings between alpha protons (HA) and alpha carbons (CA). Amide protons of glycine and non-glycine residues are simultaneously decoupled without the need for data post-processing.The proposed method can be routinely employed in amide-detected protein NMR experiments. Further, this work will facilitate the assignment and analysis of large and complex intrinsically disordered proteins in solution.

Symposium : **PHYS2-2**
Recent Progresses in Physical Chemistry
Room 600B, FRI 09:25
Chair: Kiyoung Park (KAIST)

IR induced isomerization of invisible isomer (I^5) spectroscopy

Myong Yong Choi*, **Cheol Joo Moon**

Department of Chemistry, Gyeongsang National University, Korea

Conformational structures of biomolecules play crucial roles in many physical and chemical processes, including molecular recognition and hydrogen bonding in the biological systems. Particularly, the formation of an intramolecular hydrogen bond of small biomolecules plays a pivotal role in vivo due to its pronounced effects on biomolecular structure and properties. Thus, ortho-substituted phenols (oSPs) are quite interesting because they have a hydroxy group that can easily form a hydrogen bond with adjacent substituents. However, oSPs, having a strong intramolecular hydrogen bonding, are usually short-lived (faster than ps) and/or geometrically distorted in the excited states such that the conformers are rarely observed in the excited spectrum by nanosecond laser systems. We have recently developed an IR spectroscopic technique, called IR induced isomerization of invisible isomer (I5) spectroscopy, that reflects a population transfer induced by intramolecular vibrational energy redistribution (IVR) from invisible conformers to other long-lived (slower than ns) conformers using a typical nanosecond laser system. This is another powerful gas-phase spectroscopic technique that monitors the structures of conformers with an extremely short excited state lifetime, of which spectral bands are broadened due to the energy-time uncertainty principle using ultrashort (faster than ps) pulse laser systems. We investigated the conformational structures of oSPs, such as 2-aminophenol (2-AP), 2-hydroxyformanilide (2-HFA), and 2-acetaminophenol (2-AAP) through experimental and theoretical studies of the jet-cooled target molecules in the gas phase. In particular, oSPs were jet-cooled in the molecular beam by supersonic jet expansions and investigated using a combination of quantum chemical calculations and various laser spectroscopic techniques, such as mass-selected one-color resonance two-photon ionization (R2PI), UV-UV hole-burning (UV-UV HB), and IR-dip spectroscopy. [1, 2] In this work, we have observed the spectral features of the short-lived conformers of oSPs by I5 spectroscopy for the first time. The details of I5 spectroscopy for oSPs will be presented.

Symposium : **PHYS2-3**
Recent Progresses in Physical Chemistry
Room 600B, FRI 09:50
Chair: Kiyoung Park (KAIST)

Development of Cutting-edge Mass Spectroscopic Techniques and Their Applications

Chan Ho Kwon*, Yu Ran Lee[1], Sung Man Park

Department of Chemistry, Kangwon National University, Korea
[1]*New and Renewable Energy Research Center, Ewha Womans University, Korea*

In this symposium, I will introduce the cutting-edge mass spectroscopic techniques based on mass spectrometry and laser spectroscopy developed in the lab and the experimental results achieved by utilizing those techniques. We developed the high-resolution one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) mass spectrometer, which could easily determine the precise conformational structures as well as adiabatic ionization energies of abnormal chemical species, which are analyzed based on the potential energy surfaces constructed along the conformational coordinates at the density functional theory levels. Further, the IR laser desorption and VUV laser photoionization technique being applicable to non-volatile molecular system such as biological molecules and organic complexes, was grafted onto the VUV-MATI mass spectrometer. Now, we could measure the one-photon VUV photoionization efficiency curves of non-volatile organic molecules in the gas phase desorbed from carbon powder by IR laser, which will be a versatile mass spectroscopic technique to study the conformational chemistry on numerous molecular systems.

Symposium : **PHYS2-4**

Recent Progresses in Physical Chemistry

Room 600B, FRI 10:15

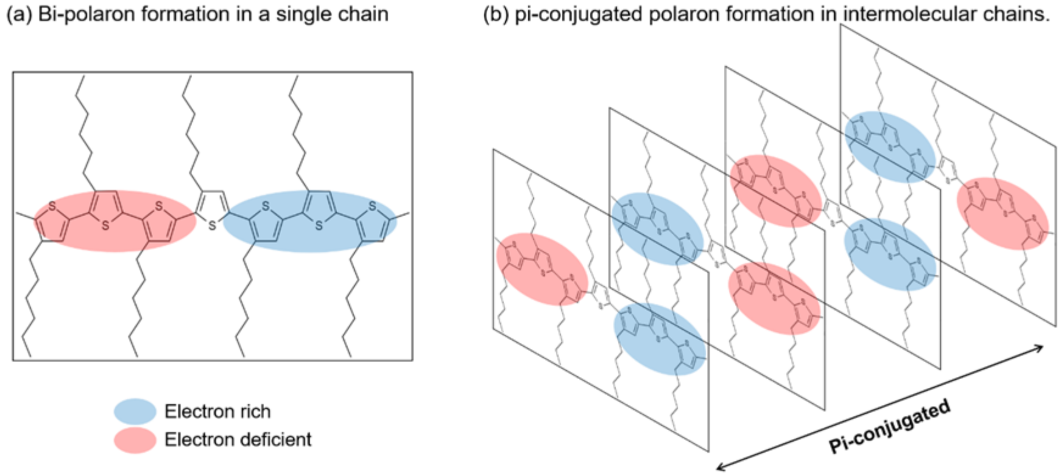
Chair: Kiyoung Park (KAIST)

Structure Studies of Poly(3-hexylthiophene) (P3HT) Using Femtosecond Stimulated Raman Spectroscopy and Computational Chemistry

Myeongkee Park

Department of Chemistry, Dong-A University, Korea

Highly pi-conjugated poly(3-hexylthiophene) (P3HT) shows an effective formation of polaron, which is critical in organic photovoltaic performance. In our theoretical and experimental studies, this polaron generation can be stimulated by a highly oscillating vibrational motion of C=C. We exploited excited-state femtosecond stimulated Raman spectroscopy (FSRS) and found the two prominent Raman peaks at ~1450 (C=C stretching) and 1350 cm^{-1} (C-C stretching) which are ~20 cm^{-1} red-shifted from ground-state Raman peak locations. This red-shift dynamics is a pure excited-state reaction which occurs within 5 picoseconds after the excitation. Using density functional theory, we have correlated the redshifts to asymmetric or half-symmetric C=C and C-C stretches, not the entire symmetric stretching modes vibrating along the whole chain. Additionally, we also have found the elongated C=C motion can effectively increase the electron density localization and shortened C=C does vice versa. Thus, this motion can effectively initiate the formation of intramolecular polarons, supporting that *the nuclear wave packet motions and electron densities are strongly correlated in P3HT* .


(a) Bi-polaron formation in a single chain

(b) pi-conjugated polaron formation in intermolecular chains.

Symposium : **PHYS3-1**
Recent Trends in Theoretical and Computational Chemistry
Room 600B, FRI 14:30
Chair: Jae Woo Park (Chungbuk National University)

Computer Simulation Studies on Soft Matter

Bong June Sung

Department of Chemistry, Sogang University, Korea

Soft matter (including polymers, colloids, surfactants, and liquid crystals) is indispensable in our daily life and modern industry. For example, slime (so called 액체 괴물) is such a popular toy for school children that there are many YouTube channels. Cosmetic products are made mostly of gels and creams. Liquid crystals and photo-reactive polymers are important materials for producing displays and semiconductors. Soft matter is also a system of academic interest due to its unique character: soft matter may behave like either liquids or solids depending on the spatiotemporal scales. For example, polymer melts flow like liquids at long time scales but are still elastic like solids at short time scales. Such a unique character makes the multiscale nature and non-equilibrium dynamics of soft matter essential topics when trying to understand and design soft matter. Over the past decades, the computer simulations have proven to be a powerful tool to investigate soft matter at many spatiotemporal scales. In this talk, I would like to share the molecular simulation studies of my group to understand the non-equilibrium nature, the phase transition, and the reaction kinetics of various soft matter systems.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **PHYS3-2**
Recent Trends in Theoretical and Computational Chemistry
Room 600B, FRI 15:00
Chair: Jae Woo Park (Chungbuk National University)

Trends in quantum computational chemistry

Joonsuk Huh

Department of Chemistry, Sungkyunkwan University, Korea

Molecules are the most prominent systems to be explored by quantum computers because they carry intrinsic quantum natures, and the corresponding quantum mechanical calculations are demanding. In my talk, I will present the recent developments in the quantum computation for chemical problems.

Symposium : **PHYS3-3**
Recent Trends in Theoretical and Computational Chemistry
Room 600B, FRI 15:20
Chair: Jae Woo Park (Chungbuk National University)

Combined theoretical and experimental studies on C-H activation reactions by metal-oxo species;not as simple as you thought.

Kyung-Bin Cho

Department of Chemistry, Chonbuk National University, Korea

C-H activation reactions are often the first step in biologically relevant substrate oxidation step, such as in hydroxylation reactions. This step is usually also the rate-limiting step, hence all the experimentally observed kinetics are dependent on the reaction rate of this particular step. Yet calculating this step with electronic structure methods is not as simple as it seems. For instance, if the catalyst is a metal-oxo species, they may have the ability to exist in several energetically close lying electronic configurations. They may hence change their electronic configuration to an optimal spin configuration for the reaction in question. Sometimes the electronic configuration changes are within the same spin state. Particularly, we found theoretically that Mn(IV)O species may utilize what we term excited state reactivity (ESR) in order to speed up the reaction. The presentation will be about our work in this general area, and also about potential reaction mechanisms beyond the initial C-H activation step.

Symposium : **PHYS3-4**

Recent Trends in Theoretical and Computational Chemistry

Room 600B, FRI 15:40

Chair: Jae Woo Park (Chungbuk National University)

Investigating a protein-ligand interaction using molecular surfaces described by three-dimensional Zernike Descriptors

Woong-Hee Shin

Department of Chemical Science Education, Suncheon National University, Korea

Recently, investigating a protein-ligand interaction using computational chemistry methods have been highlighted for drug discovery. Virtual screening is one of the popular methods to find drug candidates from a huge compound library in a short time. To predict the interaction between the molecules, most of the virtual screening methods employ an atomic model. However, the model has two disadvantages. First, calculating interactions using pairwise atomic distance takes a long time, which is not desirable for virtual screening. Second, handling molecular flexibility is hard, which requires high degrees of freedom.To overcome the hurdles, we recently developed a virtual screening method using molecular surfaces. The molecule surface is divided into a couple of overlapped patches. Chemical characteristics of the patches are encoded by a vector, called three-dimensional Zernike descriptors. The complementarity between a receptor pocket and a ligand is computed by comparing the vectors, enabling a fast search for a huge compound library. In this presentation, a key algorithm of the three-dimensional Zernike descriptors is covered and also successful applications to the real-world problem are also discussed.

Symposium : **PHYS3-5**
Recent Trends in Theoretical and Computational Chemistry
Room 600B, FRI 16:00
Chair: Jae Woo Park (Chungbuk National University)

Extending graph convolutional neural network for predicting molecular properties

Hyun Woo Kim, Gyoung S. Na, Hyunju Chang[*]

Chemical Data-driven Research Center, Korea Research Institute of Chemical Technology, Korea

The prediction of molecular properties from big-data is the most naive application of machine learning algorithms in the chemical research community. To this end, we should teach machines to recognize molecules with meaningful numbers, usually called features. These features are generated based on its composition and structural information. Conventional machine learning algorithms such as fully-connected neural network (FNN) utilize one dimensional feature vector for each molecule. In contrast, graph convolutional neural network (GCN) provides a natural representation of molecules by describing atoms and chemical bonds with nodes and edges in the graph, respectively. It was reported that GCNs show improved performance on predicting chemical reactivity and molecular properties. However, GCN is limited in treating global information of molecules. Here, we will present computational analysis on GCNs for predicting molecular properties and a possible remedy for overcoming their limitation. We will briefly introduce FNN and GCN and then explain the limitation of GCN by showing an example of ring-shape compounds. By using structural information of the whole molecule, we can propose extended GCNs with improved performance. Future applicability of newly proposed GCNs will also be discussed.

Symposium : **ANAL1-1**

[KCS-JAIMA Joint Symposium] Analytical Chemistry with JAIMA: Biosensor Development

Room 600A, THU 10:00

Chair: Jeongkwon Kim (Chungnam National University)

Design of nanocarbon film electrodes with extended analyte zones

Dai Kato

Biomedical Research Institute, National Institute of Advanced Industrial Science and Technology, Japan

We have been studying nanocarbon film electrodes formed by an electron cyclotron resonance (ECR) sputtering or an unbalanced magnetron (UBM) sputtering method.1) The film provides a nanocrystalline sp^2 and sp^3 mixed bond structure with an atomically flat surface (surface roughness of 0.05 – 0.1 nm) and high conductivity without doping. The film electrode has excellent properties including a low background current, a wide electrochemical potential window, and little surface fouling, while maintaining relatively high electrode activity for various analytes. These characteristics allow the detection of various analytes, which are difficult to measure at the conventional carbon electrodes. For example, this film electrode can measure all DNA bases (including DNA base derivatives e.g., 5'-methylcytosine) quantitatively.2) Moreover, due to their good electrochemical stability and low background current, the nanocarbon film electrode is suitable for long-term analysis including as the electrode of an HPLC detector for detecting cerebral gliotransmitter from real samples.3)

The nanocarbon film surface can be easily modified with other atoms/nanoparticle without losing its ultraflatness.4) For example, we previously developed electrochemically stable fluorinated nanocarbon (F-nanocarbon) film by CF$_4$ plasma treatment. We applied for quantitative measurements of lipophilic antioxidants (α-tocopherol) with maintaining the suppression for the responses of hydrophilic antioxidants (ascorbic acid) in liquid food samples. We observed irreversible oxidation peaks for vitamin E, but electrochemical response for vitamin C was effectively suppressed. Moreover, even in the mixed solution, the peak current at the F-nanocarbon film electrode was in good agreement with that for the vitamin E alone.5) These results indicate that there is no interference. This is highly advantageous in terms of constructing a simple assay of antioxidant because an extraction process is usually required prior to the conventional assay.

Our sputtering method can also be applied to develop metal nanoparticle-embedded nanocarbon film electrodes by using UBM co-sputtering methods for detecting some analytes (geosmin, arsenic ions and sugars), which are difficult to detect at the nanocarbon film itself.6) For example, the co-sputtering of Pt and carbon formed Pt nanoparticle (typically 2.5 nm in diameter) spontaneously in the carbon films, owing to the poor intermiscibility of Pt with carbon. With the optimized condition, we achieved excellent performance for detecting geosmin with high sensitivity solely by direct oxidation.

The most significant and implicative point of these works, is that the nanocarbon film-based electrodes can expand possibility to detect analytes, which is previously unattainable for measurements (due to electrode problem such as narrow potential window, large background noise, and low electrode activity).

References

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Symposium : **ANAL1-2**
[KCS-JAIMA Joint Symposium] Analytical Chemistry with JAIMA: Biosensor Development
Room 600A, THU 10:20
Chair: Jeongkwon Kim (Chungnam National University)

Reaction monitoring researches by using hyperpolarized parahydrogen

Keunhong Jeong

Department of Chemistry, Korea Military Academy, Korea

NMR (Nuclear Magnetic Resonance) has been harnessed as the key spectroscopic technology in both industry and science field. However, the high cost and effort of implementation and maintenance of NMR/MRI (Magnetic Resonance Imaging) due to the difficulty in maintaining strong magnetic field and cryogenic condition were the problematic even those great advantages. The best way to overcome these drawbacks is to take advantage of hyperpolarization effect that leads to the beyond the Boltzmann distribution, allowing lowered demand for strong magnetic field. Dynamic nuclear polarization (DNP) has been one of the most widely used method to induce hyperpolarization on target materials. However, DNP exhibits low efficiency and poor stability due to its harsh condition such as strong magnetic field and cryogenic condition. Furthermore, reaction monitoring application is not possible due to its low temperature condition. Therefore, there has been much efforts to induce hyperpolarization on targets using safe materials at room temperature. Several emerging tools (NV Center in diamond, 129Xe) that can induce hyperpolarization in normal condition will be introduced. After that, parahydrogen system, which is currently set up in Korea Military Academy will be introduced and several reaction monitoring research results by using hyperpolarized parahydrogen will be shared.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **ANAL1-3**
[KCS-JAIMA Joint Symposium] Analytical Chemistry with JAIMA: Biosensor Development
Room 600A, THU 10:40
Chair: Jeongkwon Kim (Chungnam National University)

Rapid and Sensitive Endotoxin Analyzer using Bioluminescence Reagents

Hiromitsu Hachiya

, DKK-TOA CORPORATION, Japan

Endotoxin is a component of the cell wall in the outer membrane of gram-negative bacteria that causes fever or shock when it enters the human blood stream.

In Japan, the concentration of endotoxins in both pharmaceutical and dialysis solutions have been regulated as shown in the following Table 1.

Limulus amebocyte lysate (LAL) is a coagulation system that is introduced by endotoxins. There are several endotoxin detection methods employing the so-called Limulus reaction using LAL. In conventional endotoxin analyzers, endotoxin detection methods using turbidimetric and chromogenic end-points as well as turbidimetric and chromogenic kinetic methods have been using. However, the two end-point methods have problems with their sensitivities (detection limits are 0.01-0.1EU/mL), and the kinetic methods have a problem with the measurement time (over 60 min).

Bioluminescence detection method has a high S/N ratio compared with other optical detection methods, such as fluorescence or chromogenic detection methods. The rapid and highly sensitive endotoxin detection method based on the bioluminescence test using mutant firefly luciferase[1)] with Limulus reaction was developed.[2)]

DKK-TOA developed the new endotoxin analyzer based on this bioluminescence detection method with Limulus reaction. The detection limit and measurement time is 0.0003 EU/mL and 20 minutes, respectively. The good performances including rapid and highly sensitive measurements were observed in the new endotoxin analyzer.

The ability of endotoxin measurement in dialysis solution was also tested by a third party and reported to be in compliance with the regulation in Japan.[3)] This analyzer has been used in many dialysate measurement sites in Japan.

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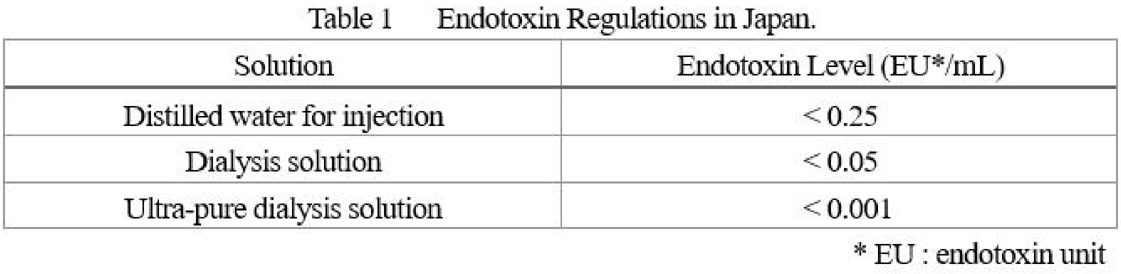

Table 1　Endotoxin Regulations in Japan.

Solution	Endotoxin Level (EU*/mL)
Distilled water for injection	< 0.25
Dialysis solution	< 0.05
Ultra-pure dialysis solution	< 0.001

* EU : endotoxin unit

Symposium : **ANAL1-4**
[KCS-JAIMA Joint Symposium] Analytical Chemistry with JAIMA: Biosensor Development
Room 600A, THU 15:40
Chair: Jeongkwon Kim (Chungnam National University)

Coulometric ion-sensor

Yumi Yoshida

Molecular Chemistry and Engineering, Kyoto Institute of Technology, Japan

Most of the ion sensors are a potentiometric device of a two-electrode system. The potentiometric device has disadvantages of potential drift and low reproducibility, and the calibration procedure is often required before the measurement. However, calibration is not suitable for point of care testing with a handy device by a non-expert person such as a customer. In the present work, we developed the thin layer electrolysis cell for the ion transfer at the liquid-liquid interface and applied it to the coulometric determination of a redox-inert ion, which works as a calibration-free ion sensor[1-4]. The thin layer electrolysis cell is a two-electrode system and has a laminate structure composed of the conducting polymer-coated electrode (CP-E), the organic thin layer membrane of 2-nitrophenyl octyl ether (NPOE, thickness of 30 μm), the aqueous thin layer solution (W, thickness of 50 μm) and an Ag/AgCl electrode (Figure 1).
We applied the thin layer electrolysis cell to the flow injection analysis of the redox-inert ion (Figure 1). The electrical charge of the current peak was converted to the mole amount through Faraday's low. In the concentration range of 5-100 μM, the electrolysis efficiency, ε%, was close to 100%, which means that the flow injection analysis in the range realizes coulometric determination (calibration-free).

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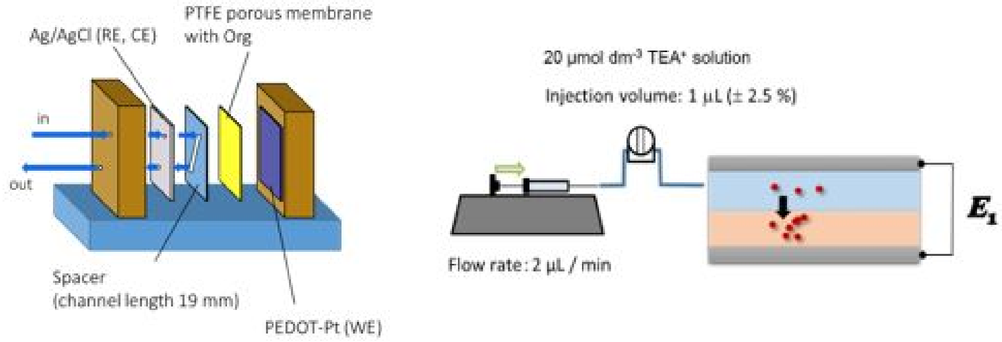

Figure 1. Scheme of coulometric determination of a redox-inert ion (tetraethylammounium cation, TEA$^+$) with the thin layer electrolysis cell for the ion transfer at the liquid-liquid interface.

Award Lecture in Division : **ANAL2-5**
Advanced In-situ/Operando Analysis for Energy and Environmental Applications
Room 600A, THU 17:20
Chair: Jaeick Lee (KIST)

A Marriage of Modern Mass Spectrometry with other Technologies: A Focus on the Lab-Automation

Han Bin Oh

Department of Chemistry, Sogang University, Korea

Recently, a focus of research in my laboratory has been given to the lab-automation. For this purpose, several technical areas have been introduced and implemented in the lab, which includes 3D-printing, milling maching, hardware controlling through arduino, software coding, and machine learning. With this, several new equipments have been built in the laboratory, for example, a sample MALDI-spotter, digital microfulidics chip system, lab-on-a-disc system, and liquid handling robot. Very recently, based on these systems, a digital ion-trap mass spectrometer is being built, which utilizes advanced FPGA and DDS (direct digital synthesis) technologies. Furthermore, based on the experience learned during these development, a new course for the undergrduate education is also being introduced and polished. The details of these trials and efforts will be given in the symposium.

Award Lecture in Division : **ANAL2-6**
Advanced In-situ/Operando Analysis for Energy and Environmental Applications
Room 600A, THU 17:40
Chair: Jaeick Lee (KIST)

From Physical Chemistry to Analytical Chemistry with NMR

Hyun Namgoong

R&D Division, KOLON, Korea

The very versatile physico-chemical tool, NMR spectroscopy, has a wide range of applications for both industrial and academic purpose. Base on physics, NMR methodology has contributed not only to investigation of chemical structure and dynamics but also to the magnetic resonance image in biological system. Multinuclear magnetic resonance measurement enables us to get the useful chemical information on nearly every element in the Periodic Table in a qualitative way. Recent development techniques such as Q-NMR as well as homo/hetero ERETIC give us to determine the absolute concentration of specific nuclei of the given molecules in a ppm level. These quantitative methods have the advantage over the other analytical tools in that there is no need to do the delicate pre-treatment experiment before measurement. Along with these analytical applications, 2-dimensional separation methodology in NMR [DOSY, ROSY] similar to chromatography can be now utilized in order to figure out the detailed structure of each component in the mixture and morphology of the polymer. In this presentation I will show how the various solution and solid NMR techniques can be applicable to real polymers in order to solve the current industrial technology issues in regard to colorless polyimide, photoresist, polyamide elastomer, which are important to foldable display, next generation car as well as eco-friendly polymer development.

Symposium : **ANAL2-1**

Advanced In-situ/Operando Analysis for Energy and Environmental Applications

Room 600A, THU 16:00

Chair: Jongwoo Lim (Seoul National University)

Nansoscale Surface Analysis for Investigation of Chemical Engineering on 2D materials

Hyunseob Lim

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

Research interest into two dimensional (2D) materials other than graphene has recently become intense, first because of the basic desire of researchers to explore new worlds in two dimensions from the point of view of materials research, and second to avoid the drawbacks of graphene for certain applications. Compared to metallic property of graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDs) have insulating and semiconducting properties, respectively. Therefore, these 2D materials can be widely used for various applications regarding to their unique properties.Herein, I present our recent research results working on graphene, h-BN and TMDs.(1-4) The presentation includes nanoscale surface analysis for investigating the chemical engineering on 2D materials. Especially, our new approaches for the periodic hydroxylation on epitaxial graphene resulting in 2D alcohol, graphenol (C6OH), and for the electrochemical surface modification on MoS2 for modulating optical transition in 2H-MoS2 are introduced. 1. Kim, G.; Kim, M.; Hong, S.; Hyun, C; Ma, K. Y.; Shin, H. S.*; Lim, H.*, ACS Nano 10, 11156. (2016)2. Jang, A.-R.; Hong, S.; Hyun, C.; Yoon, S. I.; Kim, K.; Jeong, H. Y.; Park, S. O.; Wong, K.; Kwak, S. K.; Park, N.; Yu, K.; Choi, E.; Lim, H.*; Shin, H. S.*, Nano Lett. 16, 3360 (2016).3. Lim, H.;. Jung, J.; Ruoff, R. S.; Kim, Y., Nat. Commun. 6, 8601 (2015). 4. Kim, G.(§); Lim, H.(§); Ma, K. Y.; Jang, A.-R.; Ryu, G. H.; Jung, M.; Shin, H.-J.; Lee, Z.; Shin, H. S, Nano Lett. 15, 4769 (2015). (§ equally contributed to this work)

Symposium : **ANAL2-2**
Advanced In-situ/Operando Analysis for Energy and Environmental Applications
Room 600A, THU 16:20
Chair: Jongwoo Lim (Seoul National University)

Electrochemical & Spectroscopic Analyses to Probe Intercalation of Magnesium Ions into Layered Hosts

Hyun Deog Yoo

Department of Chemistry, Pusan National University, Korea

Magnesium rechargeable batteries potentially offer high energy density, safety, and low cost due to the ability to employ dendrite-free and earth-abundant magnesium metal as the negative electrode. In addition to the ultrahigh capacity of Mg metal anode, maximum two-electron transfer per site of cathode materials can effectively enhance the capacity of the cathode. Despite recent progress, further development remains stagnated mainly due to the sluggish scission of magnesium−chloride bond and slow diffusion of divalent magnesium cations in cathodes. Due to the sluggish intercalation of Mg2+ ions, it is essential to probe genuine intercalation of Mg2+ by rigorous electrochemical & spectroscopic analyses. Here we report such endeavors in line with developing strategies for more facile intercalation of Mg2+ in sulfide and oxide hosts. First, combined theoretical modeling, spectroscopic analysis, and electrochemical study reveal fast diffusion kinetics of magnesium cation in the expanded interlayer. Even faster intercalation and diffusion kinetics were observed for magnesium monochloride ions because of the alleviated electrostatic force between S anion and Mg cation, circumventing the energy barrier due to the scission of magnesium−chloride bond. Second, multimodal characterization confirmed genuine intercalation of Mg2+ into vanadium oxide (V2O5), by probing the elemental, redox and morphological changes undergone by the oxide at 110 °C. After the thermo-electrochemical activation at high temperature operation, the electrochemical activity at room temperature was significantly enhanced by in-situ evolution to nanostructure. These strategies renew prospects for functional Mg rechargeable batteries surpassing the levels of energy density of current Li-ion batteries.

Symposium : **ANAL2-3**

Advanced In-situ/Operando Analysis for Energy and Environmental Applications

Room 600A, THU 16:40

Chair: Jongwoo Lim (Seoul National University)

In situ observation of Li–O_2 electrochemical reactions using electrochemical atomic force microscopy

Hye Ryung Byon

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

Despite more than 3 times higher theoretical energy density than that of lithium-ion batteries, lithium–oxygen (Li–O_2) batteries have not yet been used in practical applications due to a significant overpotential required for charging process (Li_2O_2 (s) → $2Li^+ + O_2 + 2e^-$ on the positive electrode). The formation and decomposition of Li_2O_2 take place during discharging and charging process, respectively, while these reactions are very sluggish due to poor electronic and ionic conductivities of Li_2O_2. In particular, Li_2O_2 decomposition process is a key hurdle for improving round-trip efficiency in Li–O_2 batteries, which was not clearly addressed. Here I show in-situ imaging of Li–O_2 redox reaction on highly oriented pyrolytic graphite (HOPG) electrode in ether-based electrolyte using electrochemical atomic force microscopy (ECAFM). For discharging, a thin film of Li_2O_2 with ~ 3 nm of thickness is deposited from edge planes of HOPG. For charging, the film decomposes at the local thinner part by ~3.7 V (vs. Li/Li^+), followed by full decomposition over 4.2 V. In comparison with such a sluggish decomposition process, the effect of redox mediator that promotes anodic behavior of Li_2O_2 is also demonstrated using ECAFM.

Symposium : **ANAL2-4**

Advanced In-situ/Operando Analysis for Energy and Environmental Applications

Room 600A, THU 17:00

Chair: Jongwoo Lim (Seoul National University)

Electrochemical Reaction Studied by In-Operando Heterodyne IR-Vis Sum Frequency Generation Spectroscopy

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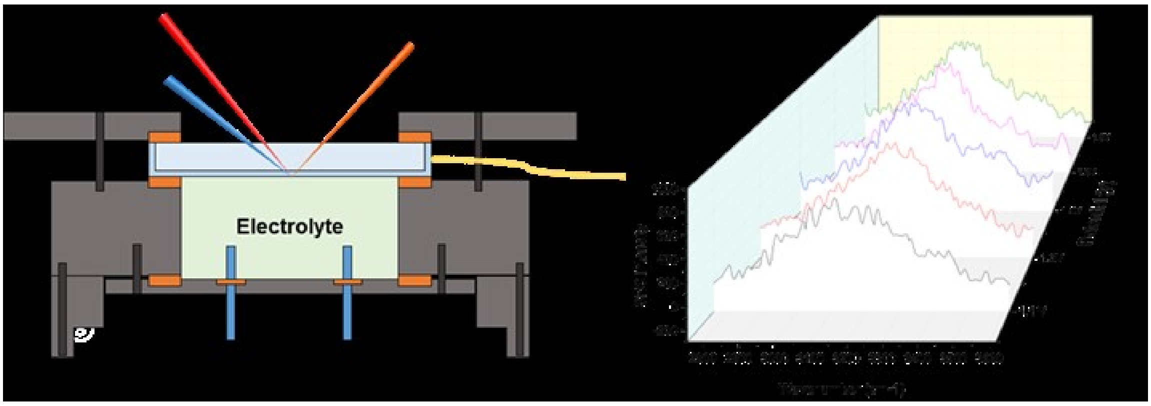
Department of Chemistry, Korea University, Korea, CMSD, IBS-Korea University, Korea, Korea

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

The surface specificity of SFG process arises from the second-order nature of the response. Under the dipole approximation, the second order response is forbidden in media with inversion symmetry. At interface or surface without inversion center, sum frequency generation process is allowed. In vibrational sum frequency generation (VSFG) experiment, we use broad band mid IR pulse (FWHM: ~250 cm-1) for vibrational excitation of surface molecules and monochromatic 800 nm pulse for up-converting mid IR. These mid IR pulse and 800 nm pulse are coincident in time and space at interface to generate sum frequency signal. This sum frequency signal is only generated when surface molecule resonant with input mid IR frequency. VSFG spectroscopy enables to measure molecular vibrations in sub-molecular layers. So vibrational sum frequency spectroscopy is suitable technique for measuring of vibrational spectrum of molecules at surfaces or interfaces. Water oxidation is an essential reaction for energy storage such as forming of hydrogen or hydrocarbons without accumulation of by-product. This reaction consists of complex multistep reactions, which adds a considerably large overpotential to the actual process. Although many studies have been conducted on OER catalysts with low overpotential and high stability, the specific catalytic reaction mechanism has not yet been elucidated. To understand the nature of heterogeneous catalytic reaction mechanism, it is important to use surface/interface selective spectroscopic method. Here, using vibrational sum-frequency generation (VSFG) spectroscopy, we selectively identified electrode-electrolyte interfacial molecules. And we designed spectro-electrochemical (SEC) cell for in situ SFG experiment. In this work, using nonlinear spectroscopic method, we can observe that the hydrogen bonding network of the interfacial water molecules changes at each potential.


Electrolyte

Symposium : **ANAL3-1**
Recent Trends in Mass Spectrometry
Room 600A, FRI 10:00
Chair: Jae-Min Lim (Changwon National University)

Exosome isolation from human serum using different centrifugation speeds

Jeongkwon Kim

Department of Chemistry, Chungnam National University, Korea

Exosomes are nanosized vesicles commonly found in biological fluids. Changes in the morphology and/or concentration of exosomes in the bloodstream can be related to specific disease stages and may be used to estimate cancer status. Exosome enrichment using ultracentrifugation at a speed of around 100,000xg is currently the most commonly used exosome enrichment method. In this study, the effect of different centrifugation speeds was investigated. The isolated exosomes were analyzed using the field emission-scanning electron microscope (FE-SEM), bicinchoninic acid assay (BCA assay), 1-D gel separation, western blotting, matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) and matrix-assisted laser desorption/ionization Fourier transform ion cyclotron resonance (MALDI-FT-ICR MS). The size distribution and protein amounts of exosomes were confirmed by FE-SEM and BCA assay.

Symposium : **ANAL3-2**

Recent Trends in Mass Spectrometry

Room 600A, FRI 10:20

Chair: Jae-Min Lim (Changwon National University)

Human Cancer Biomarker Discovery with Proteomics

Wonryeon Cho

Department of Bio-nanochemistry, Wonkwang University, Korea

Targeted proteomics using affinity chromatography (AC) has been used for identifying and quantifying cancer-related proteins through cancer and normal plasma on breast, colon, and lung cancer. Some proteins were found to be potential cancer marker candidates based on their elevation in various cancer patients. Recently, exosomes from lung cancer plasma were used to identify exosomal proteins. Exosomes are cell-derived nanovesicles that are rich source of novel biomarkers in the diagnosis and prognosis of disease. Exosomes were individually extracted from 46 patients plasma of lung cancer through size-exclusion chromatography. Each exosome sample was pooled into three TNM groups. Each group samples were analyzed multiple times on nLC-MS/MS system with various methods for exosomal protein identification from lung cancer plasma.

Symposium : **ANAL3-3**

Recent Trends in Mass Spectrometry

Room 600A, FRI 10:40

Chair: Jae-Min Lim (Changwon National University)

Laser desorption/ionization (LDI) mass spectrometry based on nanomaterials for biomedical applications

Jae-Chul Pyun

Dept. Materials Science and Engineering, Yonsei University, Korea

In conventional MALDI-TOF mass spectrometry, analyte molecules are known to be ionized by mixing with organic matrix molecules. As the organic matrix molecules are ionized, they generate unreproducible mass peaks such that MALDI-TOF mass spectrometry is nearly impossible in the low mass-to-charge (m/z) range (< 1000). In this work, we present laser desorption/ionization (LDI) mass spectrometry based on solid-matrices for the detection of small biomolecules in the low m/z range by using MALDI-TOF mass spectrometry: (1) Top-down synthesized TiO2 nanowires were synthesized as arrays using a modified hydrothermal process directly on the surface of a Ti plate; (2) The nylon nanoweb with TiO2 particles was prepared by the simultaneously electrospinning a nylon nanoweb and electrospraying TiO2 nanoparticles; (3) The parylene-matrix chip was fabricated by the deposition of nano-porous parylene-N thin film on a dried organic matrix array. The biomedical application of LDI mass spectrometry was demonstrated for (1) the detection of chemical and biological warfare agents, (2) the newborn metabolite analysis, (3) the antibiotics-resistant bacteria screening and (4) search for biomarkers for medical diagnosis of sepsis.

Symposium : **ANAL3-4**

Recent Trends in Mass Spectrometry

Room 600A, FRI 14:30

Chair: Jae-Min Lim (Changwon National University)

Deuterium-Free, Three-Plexed Peptide Diethylation for Highly Accurate Quantitative Proteomics

Jae Hun Jung, Jong-Seo Kim[1,*]

Department of ophthalmology, Yonsei University, Korea
[1]*Seoul National University, Korea*

The deuterium, a frequently used stable isotope in isotopic labeling for quantitative proteomics, could deteriorate the accuracy and precision of proteome quantification owing to the retention time shift of deuterated peptides from the hydrogenated counterpart. We introduce a novel three-plexed peptide "diethylation" using only 13C isotopologues of acetaldehyde and demonstrate that the accuracy and precision of our method in proteome quantification are significantly superior to the conventional deuterium-based dimethylation labeling in both a singleshot and multidimensional LC−MS/MS analysis of the HeLa proteome. Furthermore, in time-resolved profiling of Xenopus laevis early embryogenesis, our 3-plexed diethylation outperformed isobaric labeling approaches in terms of the quantification accuracy or the number of protein identifications, generating more than two times more differentially expressed proteins. Our cost-effective and highly accurate 3-plexed diethylation method could contribute to various types of quantitative proteomics applications in which three of multiplexity would be sufficient.

Symposium : **ANAL3-5**
Recent Trends in Mass Spectrometry
Room 600A, FRI 14:50
Chair: Jae-Min Lim (Changwon National University)

A single-injection with pre-column derivatization LC-MS/MS method for plasma metabolites

Kwangyoul Kim

Clinical pharmacology, Inha University, Korea

Metabolomics is a powerful emerging technology for studying the systems biology and biomarker discovery for various diseases. Targeted metabolomics, which focuses on the analysis of specific metabolites from biologically relevant metabolic pathways, can facilitate an overall understanding of the pathogenesis of diseases and the early diagnosis and treatment of the diseases.LC-MS/MS (MRM; multiple reaction monitoring) technique is the most widely approach used for targeted metabolomics, and features high selectivity and sensitivity, good reproducibility and wide dynamic range in quantitative analysis.Currently, targeted LC-MRM methods for polar metabolites are often limited by the number of analytes that can be measured, and/or require two or more LC platforms (HILIC or IPLC) including multiple injections.Here, we describe a selective precolumn derivatization LC-MRM based targeted metabolomics workflow for the quantitative analysis of polar metabolites, such as amino acids, biogenic amines, and carboxylic acids in central carbon metabolic pathways including an intermediate metabolite of the tricarboxylic acid (TCA) cycle.We developed a single-injection, targeted plasma metabolite quantification method on triple quadruple mass spectrometer. Analytical validation was conducted for the sensitivity, reproducibility, linearity, and carryover. The described LC-MRM method is accurate, reliable and reproducible with a wide dynamic range and also is capable of measuring polar metabolites in plasma in a single injection using small volume, resulting in significant improvement in throughput analysis.Therefore, the method might be a useful tool in helping the diagnosis of diseases and studying biomarker discovery.

Symposium : **ANAL3-6**
Recent Trends in Mass Spectrometry
Room 600A, FRI 15:10
Chair: Jae-Min Lim (Changwon National University)

Proteomic analysis of human bronchoalveolar lavage fluid towards the biomarker discovery for lung cancers

Min-Sik Kim

Department of New Biology, DIGST, Korea

Lung cancer is one of the most common cancers among many others and the leading cause of cancer-related mortality worldwide. Since the early diagnosis of the lung cancer is one of the main purposes in the field of lung cancer research, the sensitive detection of biomarker proteins from bronchoalveolar lavage fluid (BALF) has been suggested as a promising method to diagnose the lung cancer. BALF is a type of fluids that can be easily obtained from patients by endoscopically introduced device and it is believed that the process of collecting the fluid is relatively minimally invasive. Here, we aimed to develop a novel and comprehensive mass spectrometry-based method for in-depth single proteomic analysis of BALF by utilizing antibody-based depletion of relatively high abundant proteins from BALF. A total of 4,615 protein groups mapped to 4,535 gene names were identified by using LC-MS/MS from the pooled BALF sample. Our method was found to outperform conventional proteomic methods that analyzed BALF samples. Further study of multiple BALF samples from different patients to discover a list of potential biomarkers for lung cancer. I believe that this method developed in this study should expedite the lung cancer biomarker discovery.

Symposium : **LIFE1-1**
[Life Chemistry Division-Korean Peptide Protein Society Joint Symposium] Recent Trends in Peptide Chemistry
Room 301, THU 15:40
Chair: Soo Hyuk Choi (Yonsei University)

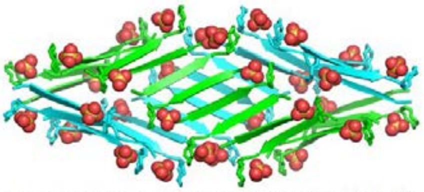
Unlocking the Mysteries of Amyloid Diseases with Macrocyclic β-Sheet Peptides & The Supramolecular Chemistry of the Antibiotic Teixobactin

James S. Nowick

Chemistry, University of California, Irvine, United States

This presentation will cover two ongoing projects in my laboratory aimed at elucidating the structures and interactions of biologically relevant peptides. The first seeks to understand the supramolecular assemblies of the oligomers formed by the β-amyloid peptide Aβ in Alzheimer's disease. The second seeks to better understand how the antibiotic teixobactin achieves its remarkable activity against Gram-positive pathogens. In the amyloid project, we have constructed a series of conformationally constrained peptides derived from Aβ and elucidated their oligomeric assemblies by X-ray crystallography. We have then generated antibodies against these assemblies and identified features in the brains from transgenic mouse models for Alzheimer's disease that react with these antibodies. In the teixobactin project, we have discovered that amyloid-like assembly of teixobactin-derived peptides generates receptors for anions, and we have provided a working model for how teixobactin binds lipid II and related cell wall precursors. Recent results and ongoing studies in both of these projects will be presented.

β-Hairpin derived from Aβ forms a trimer, dodecamer, and annular pore.



Teixobactin analogue forms a double helix of β-sheet fibrils that binds sulfate anions.

Symposium : **LIFE1-2**
[Life Chemistry Division-Korean Peptide Protein Society Joint Symposium] Recent Trends in Peptide Chemistry
Room 301, THU 16:20
Chair: Soo Hyuk Choi (Yonsei University)

Strategies for modulation of secondary structures to optimise biological recognition

Anna Maria Papini

Chemistry, University of Florence, Italy

Side chain-to-side chain cyclizations represent a strategy for enrichment of bioactive conformational ensembles. Structural rigidification reduces entropy and may lock molecules into receptor binding conformations. Anyway, structural manipulations contribute to enhance target specificity, induce higher binding affinity and biological potency, and lead very often to lower metabolic susceptibility and more favorable pharmacokinetics. The CuI-catalyzed azide−alkyne 1,3-dipolar Huisgen's cycloaddition (CuAAC) provides a convenient and versatile access to cyclic peptidomimetics following incorporation of the building blocks Nα-Fmoc-Xaa(ω-N3)-OH and Nα-Fmoc-Yaa(ω-yl)-OH. The proteolytic stable side chain-to-side chain bridging [1,2,3]triazolyl moiety in peptides, is isosteric with the peptide bond and can function as a surrogate of the classical lactam forming bridge. As a proof-of-concept we introduced the [1,2,3]triazolyl bridge in a PTHrP model cyclopeptide demonstrating that i-to-i+4 side chain-to-side chain cyclization offers a powerful approach for generating stable helix mimetic structures. Then we demonstrated that i-to-i+5 side chain-to-side chain 1,4-disubstituted [1,2,3]triazolyl-bridge can stabilize β-turn conformations in MT-II peptides. Not only the [1,2,3]-triazolyl moiety but also bridge size and its location and orientation within the bridge appear to be fundamental to mimic the biological activity. In fact, conformational and biological studies confirmed that [1,2,3]triazolyl-mediated side chain-to-side chain cyclization results in conformational stabilization of type-I β turn generating heterodetic cyclopeptides with enhanced in vitro potency and improved receptor subtype selectivity. The same approach has been also successfully used to replace the susceptible disulfide bridge stabilizing the bioactive conformational behavior of Octreotide-derived radiotherapeutics. On the other hand we demonstrated that dicarba analogs in which the bulky aromatic side chain of Tyr(Bzl) favored the formation of a 310-helix, displayed enhanced sst5 selectivity suppressing the sst2 affinity. Efficient on resin MW-assisted RCM allowed to investigate the influence of the stereochemistry of some strategic amino acids on the propensity to give the cyclic compounds in mild conditions and new DOTA-conjugated Octreotide analogs exhibited nanomolar affinities on sst2 and sst5 somatostatin receptor subtypes. Stabilization of β-turn structures was also achieved by a 1,3-butadiyne constraint via the Glaser oxidative coupling to mimic conformational epitopes in the synthetic peptide CSF114(Glc) previously designed to fold as a type I’ β-turn structure recognising specific antibodies in multiple sclerosis and Rett Syndrome. Moreover, a synthetic photochromic azobenzene amino acid derivative was introduced as a turn element to replace the P-N-H fragment at positions 7-9 (involved in the β-hairpin in the peptide analogue [Pro7,Asn8,Thr10]CSF114 previously designed to fold as a type I β-turn optimized structure to recognize antibodies. The electronic properties of the novel azopeptidomimetic analog were investigated and we verified that isomerization results strongly favored by exciting into the ππ* transition. Moreover, conformational changes induced by the cis↔ trans azopeptidomimetic switch were investigated by NMR in different solvents.

Symposium : **LIFE1-3**
[Life Chemistry Division-Korean Peptide Protein Society Joint Symposium] Recent Trends in Peptide Chemistry
Room 301, THU 17:00
Chair: Soo Hyuk Choi (Yonsei University)

Peptide-based surface-fill hydrogel facilitates miRNA delivery to treat mesothelioma

Poulami Majumder, Anand Singh[1], Caroline Andrews[2], Ziqiu Wang[3], Kingshuk Dutta[4], Nimit Patel[5], Natalia De Val Alda[3], Chuong D. Hoang[1,*], Joel P. Schneider[*]

Chemical Biology Laboratory, National Cancer Institute, National Institutes of Health, United States
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[2] *Cancer and Inflammation Program, Center for Cancer Research, National Cancer Institute, National Institutes of Health, United States*
[3] *Advanced Technology Research Facility, United States*
[4] *Department of Chemistry, University of Massachusetts Amherst, United States*
[5] *Small Animal Imaging Facility, Leidos Biomedical Research, Inc., United States*

Cancers, such as mesothelioma, that grow as sheets on the surface of organs and tissues having complex anatomical features represent a unique challenge in oncology. In contrast to solid tumor masses, their surgical resection often leaves residual cancer that causes rapid recurrence. We developed a peptide-based hydrogel that can be sprayed or injected to effectively cover large surface areas of organs and tissues having complex anatomical features, including those resulting from surgical resection. Once implanted, the material can shape-change to accommodate real-time changes in tissue morphology. The material locally delivers nanoparticles engineered from intrinsically disordered peptide and miRNA that effectively enter cells, escaping the acidic endosome to target mRNA important for the progression of mesothelioma, an aggressive asbestos-related cancer. Interestingly, endosomal release of the nanoparticles is dependent on the conformational state of the peptide comprising the particle-the peptide must be disordered. We show that with a single application, this gel produces a durable pre-clinical response in three increasingly complex models of mesothelioma. In principle, this regional treatment strategy could be applied to other surface cancers, including ovarian carcinoma and gliomas.

Symposium : **LIFE2-1**
Light Irradiation Deep into Life-Science Chemistry
Room 301, FRI 09:00
Chair: Seokhee Kim (Seoul National University)

Optical Sensing and Control of Protein Activity in Live Cells by Fluorescent Protein Technology

Jihye Seong

Brain Research Institute, KIST, Korea

Recent advances in fluorescent protein (FP) technology made a great contribution to the development of current biology field. For example, florescent molecular biosensors based on fluorescence resonance energy transfer (FRET), which can be detected between donor and acceptor FPs in proximal, provide powerful tools to visualize dynamic molecular interactions and protein activity in live cells. I will discuss how the FRET-based kinase biosensors are developed to report the real-time kinase activity at subcellular membrane compartments. I will also introduce newly developed GPCR biosensors based on circular permuted FP (cpFP). Fluorescent protein technology can be further applied to control protein activity by light. In particular, I will introduce an optogenetic strategy to control protein activity by caging the functional domain of the target protein with photodissociable Dronpa dimmer. As the caged domain can be exposed as the dimeric Dronpa became monomers by photoswitching, we can control the protein activity by light. Taken together, fluorescent proteins and advanced imaging technologies enable both optical sensing and control of target protein activity in live cells, which will be powerful tools to understand the real-time molecular events with high spatiotemporal resolutions.

Symposium : **LIFE2-2**

Light Irradiation Deep into Life-Science Chemistry

Room 301, FRI 09:20

Chair: Seokhee Kim (Seoul National University)

Quantum Dots for Imaging Applications

Sung Jee Kim

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

A few imaging applications using quantum dots (QDs) will be introduced, which will cover from visible to infrared(IR) for the wavelengths and from cellular super-resolution to whole body in vivo imaging for the object scale. (1) QDs were conjugated to tumor-specific antibodies(Abs) with zwitterionic surface coating to reduce nonspecific bindings. The Ab-QD probes were used to diagnose tumors for sectioned mouse tissues, fresh mouse colons stained ex vivo and in vivo, and also for fresh human colon adenoma tissues. The probes successfully detected not only cancers that are readily discernible by bare eyes but also hyperplasia and adenoma regions. Multiplexed QD, spray-and-wash, and endoscopy approach provided a significant advantage for detecting small or flat tumors that may be missed by conventional endoscopic examinations. QD-Ab probe was also used in conjunction with a ratiometric fluorescent molecular probe, cresyl violet–glutamic acid derivative, that ratiometrically switches between two fluorescent colors in response to the enzyme activity of λ-glutamyltranspeptidase. Co-application of the two kinds of probes, QD-Abs and the ratiometric molecular probe, afforded accurate visualization of carcinomas, hyperplasia and adenoma regions. (2) Amphiphilic polyethyleneimine derivatives (amPEIs) were synthesized and used to encapsulate dozens of QDs. The QD-amPEI showed very efficient QD cellular fluorescent labeling. Co-encapsulation of QDs and oxygen sensing phosphorescence Ru dyes allowed accurate and reversible oxygen sensing capability by the ratiometric signals, which was successfully applied to cellular and spheroid models. (3) Photo-modulating QDs were designed by conjugating crystal violets (CVs) on QD surface. The QD CV conjugates (QD-CVs) shows a single cycle of emission burst as go through the stage of initially quenched off to photo-activated on and back to photo-darkened off stage. The QD-CV probes were introduced into cells, and the visible light excitation yielded photo-modulation nearly ten folds in intracellular environment. Exploiting the stochastic PL burst of QD-CVs and multiplexing capability of QDs, simultaneous multi-color super-resolution localizations were demonstrated. (4) Recent technological advances have expanded fluorescence imaging into the second near-infrared region (NIR-II; wavelength =

1000–1700 nm), providing high spatial resolution through deep tissues. However, bright and compact fluorophores are rare in this region, and sophisticated control over NIR-II probes has not been achieved yet. We showcase an enzyme-activatable NIR-II probe that exhibits turn-on fluorescence upon matrix metalloprotease activity in tumor microenvironment.

Symposium : **LIFE2-3**

Light Irradiation Deep into Life-Science Chemistry

Room 301, FRI 09:40

Chair: Seokhee Kim (Seoul National University)

Base-pair opening dynamics study of nucleic acids by NMR spectroscopy

Joon-Hwa Lee

Department of Chemistry, Gyeongsang National University, Korea

Base-pair opening in nucleic acids is a structural fluctuation for proper conformational transitions that is required in their biological function. NMR hydrogen exchange experiment is one of widely used method to study the thermodynamics and kinetics for base-pair opening in nucleic acids. The hydrogen exchange data of imino protons are analyzed based on a two-state (open/closed) model for the base-pair, where hydrogen exchange only occurs from the open state. Here, we reported three base-pair opening dynamics studies which provide insights into the biological function of the interesting nucleic acids. First, a base-pair opening dynamics study was performed using model RNAs mimicking the cleavage site of wild type and B5 bulge-stabilizing mutant pri-miR156a constructs. This study suggests that the stabilities and/or opening dynamics of the C15·G98 and U16·A97 base-pairs at the cleavage site are essential for formation of the active conformation and for efficient processing of pri-miR156a, and that mutations of the B5 bulge can modulate mature miR156 levels as well as miR156-driven leaf number phenotypes via changes in the base-pair stability of the cleavage site. Second, the base-pair opening kinetics studies of three GATC-containing DNA duplexes found that two G·C base pairs of the hemimethylated GATC duplex displayed a faster base-pair opening rate and required less energy for the base-pair opening reaction than did those of the fully methylated one. Finally, the base-pair opening data of the P1 duplex of the Tetrahymena group I ribozyme revealed that three base pairs, U-1·G22, C-2·G23 and A2·U21 showed unusual base-pair opening thermodynamics which might be correlate with the undocking rates of the P1 helix into catalytic core.

Symposium : **LIFE2-4**

Light Irradiation Deep into Life-Science Chemistry

Room 301, FRI 10:15

Chair: Hyun-Woo Rhee (Seoul National University)

Label-free optical microscopic imaging deep within living animals

Wonshik Choi

IBS Center for Molecular Spectroscopy and Dynamics, Department of Physics, Korea University, Korea

Optical microscopy suffers from the loss of resolving power when imaging objects embedded deep within scattering media such as biological tissues. In this talk, I will present a label-free and high-resolution imaging method that can remove the sample-induced aberrations without the need for guide stars and even in the presence of multiple light scattering. Experimental results for in vivo volumetric imaging of a living zebrafish and imaging through an intact mouse skull will be presented to validate the capability of the proposed method.References [1]M. Kim et al., Nat. Commun. 10, 3152 (2019)[2]S. Kang, P. Kang et al., Nat. Commun. 8, 2157 (2017)[3]S. Kang, S. Jeong et al., Nature Photonics 9, 253 (2015)[4]S. Jeong, Y. Lee et al., Nature Photonics 12, 277 (2018)

Symposium : **LIFE2-5**
Light Irradiation Deep into Life-Science Chemistry
Room 301, FRI 10:35
Chair: Hyun-Woo Rhee (Seoul National University)

Label-free Mass Spectrometric Imaging for Biological Applications

Tae Geol Lee

Center for Nano-Bio Measurement, Korea Research Institute of Standards and Science, Korea

Recently, surface mass spectrometric analysis (and imaging) techniques such as MALDI-MS and ToF-SIMS are getting popular since they can measure chemical compositions/distributions of bio-related sample surfaces. Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) has been used for molecular identification of proteins in the discovery of disease-related biomarkers as a key platform technique in proteomics. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) on the other hand has been used to analyze small biomolecules such as amino acids, peptides, vitamins and drugs in the top-layer (1-2 nm probing depth) because the collisional cascade process cannot produce secondary ions with a molecular weight of over m/z 2,000 without the use of noble metals or MALDI matrixes. First, we will show our recent ToF-SIMS data of tissue samples obtained by using various primary ion beams and sampling methods, and discuss the potential capability of ToF-SIMS to study for –omics, particularly lipidomics for tissue study.[1-6] Second, we will show that ToF-SIMS imaging analysis of peptides enables efficient screening for enzyme inhibitors, thus permitting high-throughput drug screening with high accuracy, sensitivity and specificity.[7] Finally, a new strategy of biomolecules (microRNA and proteins) detection by using imaging mass spectrometry will be presented.[8][1] Yun et al., Anal. Chem. 83, 9298-9305 (2011)[2] Park et al., Scientific Reports, 5:11077 (2015)[3] Shon et al., Biointerphases, 11, 02A321 (2016)[4] Son et al., J. Vac. Sci. Tech. B, 34, 03H133 (2016)[5] Kim et al., J. Am. Soc. Mass Spectrom. 28:1729-1732 (2017)[6] Shon et al., Biointerphases, 13, 03B411 (2018) [7] Cho et al., Anal. Chem. 89, 799-806 (2017) [8] Na et al., submitted

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

International Symposium on Organic Chemistry: Recent Developments on C-H Activation Reactions

Convention Hall 1+2, THU 15:40

Chair: Bongjin Moon (Sogang University)

Catalyst and Reaction Development for Sustainable Chemical Synthesis from Readily Available Feedstocks

Soon Hyeok Hong

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

The development of useful, practical, and selective synthetic methods that generate minimal by-product is of critical importance in both academic and industrial research. The research of our group seeks to develop efficient and environmentally friendly synthetic methods through molecular catalysis. Specifically, we have explored novel C-N formation reactions from primary alcohols and various N-sources, chemical synthesis utilizing CO_2 and methanol as C1 sources, and development of organometallic catalysts for C-H functionalization and C-C bond formation reactions. Our past and recent approaches to the reaction and catalyst development for sustainable chemical synthesis will be presented.

Symposium : **ORGN1-2**

International Symposium on Organic Chemistry: Recent Developments on C-H Activation Reactions

Convention Hall 1+2, THU 16:10

Chair: Sunwoo Lee (Chonnam National University)

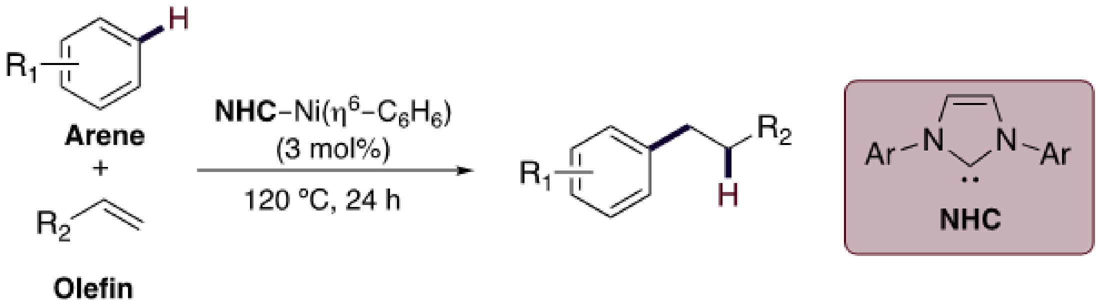
Anti-Markovnikov Hydroarylation of Alkenes Controlled by Non-Covalent Interactions

John F. Hartwig

Department of Chemistry, University of California, United States

Our research group has studied catalytic hydrofunctionalization of alkenes since we first disclosed in 2000 the additions of arylamines to vinylarenes catalyzed by palladium complexes. Since that time, we have expanded these studies to encompass nickel, rhodium and iridium catalysts and have achieved additions of C-H and N-H bonds to unactivated alkenes. Most recently, we have identified catalysts for the addition of the C-H bonds of unactivated arenes to unconjugated alkenes with anti-Markovnikov selectivity. Analysis of the mechanism of this reaction reveals an unusual C-H bond cleavage step and unexpected effects of the substituents of the ligands on the rate of the reaction. This lecture will comprise our studies on this unusual hydroarylation process.

1. Kawatsura, M.; Hartwig, J. F., Palladium-Catalyzed Intermolecular Hydroamination of Vinylarenes using Arylamines. *J. Am. Chem. Soc.* **2000**, *122*, 9546-9547.
2. Liu, Z.; Hartwig, J. F., Mild, Rhodium-Catalyzed Intramolecular Hydroamination of Unactivated Terminal and Internal Alkenes with Primary and Secondary Amines. *J. Am. Chem. Soc.* **2008**, *130 (5)*, 1570-1571.
3. Sevov, C. S.; Zhou, J.; Hartwig, J. F., Iridium-Catalyzed Intermolecular Hydroamination of Unactivated Aliphatic Alkenes with Amides and Sulfonamides. *J. Am. Chem. Soc.* **2012**, *134 (29)*, 11960-11963.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Symposium : **ORGN1-3**

International Symposium on Organic Chemistry: Recent Developments on C-H Activation Reactions

Convention Hall 1+2, THU 16:35

Chair: Sunwoo Lee (Chonnam National University)

Mechanism-Driven C-H Amidation: Reaction Development and Asymmetric Catalysis

Sukbok Chang

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

Direct amidation of C–H bonds is a highly desirable reaction considering high utility of amidated products in total synthesis, medicinal chemistry and materials science. Although tremendous research efforts have been made especially in recent years, the current status enabling such C–H reactions in excellent stereoselectivity and high efficiency is still rather limited. In this context, we have developed a novel methodology that employs tailor-made Ir-based catalysts in combination with dioxazolone substrates to access a short-lived metal-nitrenoid intermediate, thereby eventually leading to a construction of γ-lactams via an outer-sphere C–H insertion pathway. The scope was found to be broad and a range of carboxylic acids could be readily utilized for the lactam formation. Indeed, the power of this new method was demonstrated in the successful late-stage functionalization of bio-active molecules to produce molecules that are highly sought after for pharmaceutical applications. More recently, we have successfully introduced an iridium-based catalyst system for asymmetric C−H amidation that enables facile construction of chiral γ-lactams starting from commodity chemicals. Various types of secondary C−H bonds, such as being positioned at the benzylic, unactivated aliphatic, propargylic, and allylic sites, were all smoothly reacted in a regio- and stereoselective manner. The present approach will find broad applications in medicinal chemistry, and the mechanistic insights may provoke further developments in related asymmetric catalysis.

Symposium : **ORGN1-4**
International Symposium on Organic Chemistry: Recent Developments on C-H Activation Reactions
Convention Hall 1+2, THU 17:00
Chair: Sunwoo Lee (Chonnam National University)

From Hydroacylation to Organic-Inorganic Hybrid Material

Chul-Ho Jun

Department of Chemistry, Yonsei University, Korea

Transition metal-catalyzed C-H bond activation is one of current interests in organic synthesis in terms of environmentally benign reaction. Among them, hydroacylation, in which aldehyde can be transformed to ketone, draw synthetic organic chemists' attention. The important elementary step in this reaction is C-H bond activation of aldehyde to generate acylmetal hydride. However, intermolecular hydroacylation was not much successful due to the decarbonylation side reaction process of unstable acylmetal hydride intermediate. We developed successful intermolecular hydroacylation process using a mixed cooperative catalyst of Rh(I) complexand 2-amino-3-picoline to evade decarbonylation. When the reaction is carried out with alkyne instead of alkene, corresponding alph,beta-unsaturated ketone is obtained. To this reaction mixture, addition of cyclohexylamine allows to cleave triple bond of alkyne. Instead of cyclohexylamine, use of benzylamine affords ortho-alkylation as well as hydroacylation. Based on this result, orthoalkylation of aromatic ketone is successfully achieved through the formation of benzylimine intermediate. During the course of studying this chelation-assisted hydroacylation, transition metal catalyzed O-silylation process was newly developed, which is further applied to the immobilization of organic molecule onto silica or glass surface. In this process, surface hydroxy group of silica or glass reacts with vinylsilane containing organic functional group to generate organic group-immobilized hybrid material wtih the covalent siloxane bond in the presence of a mixed catalyst of Rh(I) and HCl. This process is further applied to the immobilization of enzyme onto silica surface.

Symposium : **ORGN1-5**
International Symposium on Organic Chemistry: Recent Developments on C-H Activation Reactions
Convention Hall 1+2, THU 17:25
Chair: Sunwoo Lee (Chonnam National University)

The Quest for Efficient Ligands in Asymmetric C-H Functionalizations

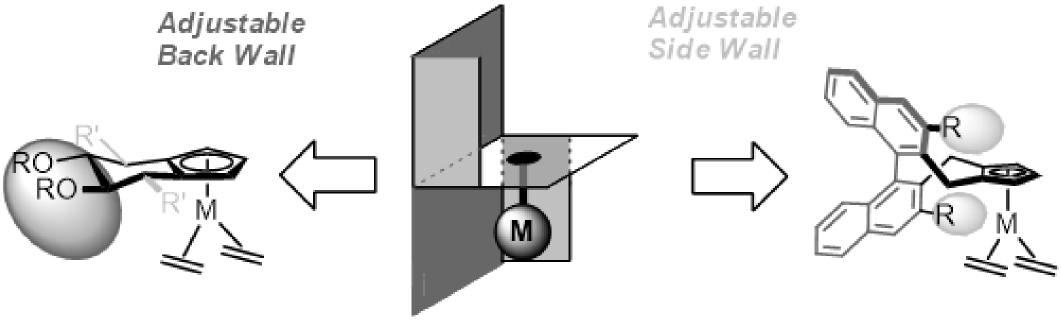
Nicolai Cramer

Laboratory of Asymmetric Catalysis and Synthesis, Institute of Chemical Sciences and Engineering, Switzerland

Reactions involving the selective activation and subsequent functionalization of C-H bonds have a high synthetic potential because of their economic and ecological benefits. Despite significant progress in addressing reactivity and selectivity issues, as well as refining mechanistic understanding of the different pathways, catalytic enantioselective transformations remain challenging.1 Often harsh conditions, the use of uncommon ligand systems or bar metal salts as catalysts have hampered developments in this area. Therefore, the design and development of efficient ligand systems is critical to the success these transformations. Over the past decade, $\mathrm{Cp^*Rh^{III}}$, $\mathrm{Cp^*Ir^{III}}$ and $\mathrm{Cp^*Co^{III}}$ complexes have emerged as extremely powerful catalysts for a very broad range of highly useful C-H functionalizations. This makes the development and engineering of the Cp ligand to an exciting task. The presentation will focus on recent developments of chiral cyclopentadienyls as ligands for catalytically competent transition-metals.2 The arising complexes are shown to be powerful catalysts for enantioselective C-H activations for a streamlined access to relevant small molecules. Aspects of ligand accessibility, complexation strategies and catalytic reactions involving mainly group 9 metals will be discussed.

References:

1. C. G. Newton, S.-G. Wang, C. C. Oliveira, N. Cramer, *Chem. Rev.* **2017**, *117*, 8908.
2. (a) B. Ye, N. Cramer, Acc. Chem. Res. 2015, 48, 1308. (b) C. G. Newton, D. Kossler, N. Cramer, *J. Am. Chem. Soc.* **2016**, *138*, 3935.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Symposium : **ORGN2-1**

Current Trends in Organic Chemistry I: Synthetic Methodology and Catalysis

Convention Hall 3, FRI 09:00

Chair: Jung Min Joo (Pusan National University)

Transition Metal-Catalyzed Alkyne Functionalization for Use in Organic Synthesis

Chulbom Lee

Division of Chemistry, Seoul National University, Korea

Transition metals interact with alkynes to form σ-alkynyl, π-alkyne and vinylidene complexes that exist in dynamic equilibrium with one another. Our laboratory has been engaged in the development of new synthetic methods that make use of alkynes via mechanisms involving a metal vinylidene as a catalytic intermediate. A diverse array of new reactions has been developed, including enyne cycloisomerizations, and various processes effecting hydrative, alkylative, and carboxylative cyclizations. Recently, in a departure from these C-C bond-forming cyclizations, our explorations have been focused on the oxygen-transfer to the metal-bound carbene intermediate. This approach has led to discovery of alkyne oxygenation that occurs through the intermediacy of a metalloketene arising from catalytic oxidation of the metal vinylidene. Discussed in this presentation will be the design, implementation and mechanistic studies of the metal vinylidene-mediated catalytic oxidative reactions of alkynes. Also presented will be a tandem addition–cyclization–rearrangement process, where alkyne- tethered hydrazones react with organoboronic acids to give cycloalkene products in a traceless fashion. The cascade reaction is based on merger of pericyclic rearrangement and transition metal mediated catalysis making use of a π-alkyne intermediate. The novel process can also be performed with enantiocontrol. Employing a chiral diene ligand for the rhodium catalyst, the reaction provides cycloalkenes with an exo stereocenter in high enantioselectivity.

Symposium : **ORGN2-2**

Current Trends in Organic Chemistry I: Synthetic Methodology and Catalysis

Convention Hall 3, FRI 09:25

Chair: Jung Min Joo (Pusan National University)

Investigation of Nickel-Catalyzed Cycloaddition Reactions

Sung You Hong

Ulsan National Institute of Science and Technology, Korea

In this talk, the reaction development and mechanistic studies of nickel-catalyzed cycloaddition reactions are presented. In particular, the origin of reactivity preference and regioselectivity of nickel-catalyzed azide–alkyne cycloaddition[1] will be demonstrated. The intermediate studies and competition experiments will be discussed.Reference:[1] Kim, W. G.; Kang, M. E.; Lee, J. B.; Jeon, M. H.; Lee, S.; Lee, J.; Choi, B.; Cal, P. M. S. D.; Kang, S.; Kee, J.-M.; Bernardes, G. J. L.; Rohde, J.-U.; Choe, W.; Hong, S. Y.* “Nickel-catalyzed azide–alkyne cycloaddition to access 1,5-disubstituted 1,2,3-triazoles in air and water” J. Am. Chem. Soc. 2017, 139, 12121–12124.

Symposium : **ORGN2-3**
Current Trends in Organic Chemistry I: Synthetic Methodology and Catalysis
Convention Hall 3, FRI 10:00
Chair: Jung Min Joo (Pusan National University)

Visible Light Photoredox-Catalyzed Deoxygenation of N-Heterocyclic *N*-Oxides

Jun Hee Lee

Department of Advanced Materials Chemistry, Dongguk University, Korea

N-Heterocycles are ubiquitous in biologically active natural, pharmaceutical, and agrochemical products, advanced functional materials, chiral ligands, and so on. Since the seminal work by Fagnou, the direct functionalization of oxygenated N-heterocyclic substrates via a C-H activation strategy has gained great popularity as a powerful synthetic tool for the controlled forging of carbon-carbon and carbon-heteroatom bonds, wherein *N*-oxide plays a key role as a superb directing group. Although several direct C-H functionalization protocols have been reported using *N*-oxide as a traceless directing group, various substituted *N*-oxide derivatives are obtained as the final product in most catalytic processes. Accordingly, deoxygenation reactions that furnish N-heterocycles in a chemoselective manner represent a fundamental transformation in organic synthesis. Despite the recent invention of several successful implementations of these reactions, such approaches commonly require the use of oxophilic reagents or intermediates under harsh reaction conditions. In this context, the development of a new method for the room temperature deoxygenation of N-heteroaromatic *N*-oxides would be useful if the otherwise labile functional groups are compatible with the reaction conditions. In our continuous efforts to develop new transformations via visible-light-induced photoredox catalysis, we recently developed a scalable and operationally simple protocol that allows for the chemoselective deoxygenation of a wide range of N-heterocyclic N-oxides at ambient temperature. The newly developed protocol features its operationally simplicity, scalability, and practicality. Further details of this useful protocol will be discussed in the presentation.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Symposium : **ORGN2-4**

Current Trends in Organic Chemistry I: Synthetic Methodology and Catalysis

Convention Hall 3, FRI 10:25

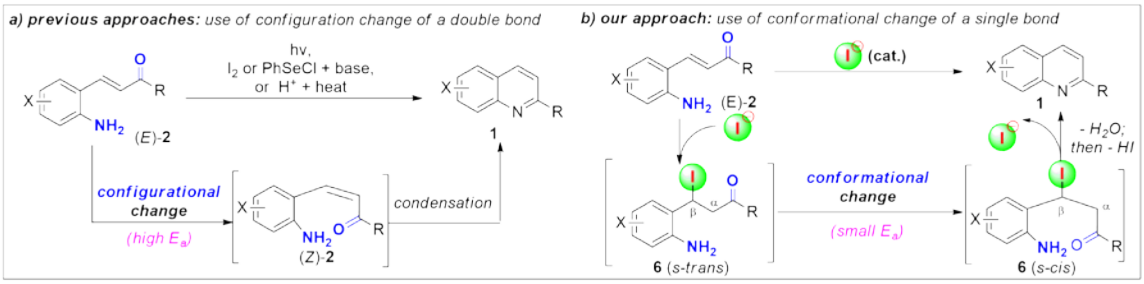
Chair: Jung Min Joo (Pusan National University)

Synthesis of Quinolines from 2-Aminochalcones Using A Nucleophile as the Catalyst

Cheol-Hong Cheon

Department of Chemistry, Korea University, Korea

Dehydrative cyclization of 2-aminochalcone derivatives 2 is one of the convenient protocols for the synthesis of 2-aryl substituted quinolines 1. However, in general, the conversion of 2 to 1 is unlikely to take place, because 2 exist in the stable (E)-configuration, where the amino group cannot approach the carbonyl group to undergo the condensation reaction. Thus, most previous methods have exploited the conversion of the stable, but unreactive (E)-configuration of 2 into the unstable, but reactive (Z)-configuration using (Scheme 1a). We envisioned that quinolines 1 could be synthesized from 2-aminochalcones 2 via dehydrative cyclization in the presence of a nucleophile capable of conjugate addition to the α,β-unsaturated carbonyl moiety present in 2 (Scheme 1b). The nucleophile could convert 2 into the corresponding saturated ketones 6 via conjugate addition of the nucleophile, and 6 could adopt the s-cis conformation where the amino and carbonyl groups can be proximally located via free rotation about the Cα-Cβ single bond. Subsequent condensation between these two groups followed by the elimination could provide the corresponding quinolines 1, with a regeneration of the catalyst. Based on this hypothesis, my research group has recently commenced with a program towards the developments of a novel approach toward the synthesis of quinolines 1 from 2-aminochalcones 2 using a nucleophile as the catalyst. In this presentation, I will present the recent progress in the synthesis of quinolines 1 via the dehydrative cyclization of 2-aminochalcones 2 using a nucleophile as the catalyst.


a) previous approaches: use of configuration change of a double bond
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I2 or PhSeCl + base,
or H+ + heat
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(high Ea)
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b) our approach: use of conformational change of a single bond
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Symposium : **ORGN3-1**

Current Trends in Organic Chemistry II: Synthetic Methodology and Total Synthesis

Convention Hall 3, FRI 14:30

Chair: Kyungsoo Oh (Chung-Ang University)

Asymmetric Syntheses of Uleine and Tubifolidine: General Approach to 2-Azabicyclo[3.3.1]nonane Indole Alkaloids

Dong-Hyun Kim, Jang Yeop Kim, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Hexahydro-1,5-methano-1H-azocino[4,3-b]indole is the pivotal structural framework that an array of Strychnos alkaloids of the strychnan and aspidopermatan types share in common. Such tetracyclic ring system is also found in the uleine type indole alkaloids including uleine, dasycarpidone and tubotaiwine. A number of elegant synthetic strategies have been developed since the first synthesis of strychnine, the most prominent member of the class, by Woodward in 1954. Those elaborations including the Woodward's are mostly based on the routes either starting with or installing the indole unit in early stage of the synthesis. The late stage indole installation approach would have notable merits including those associated with convergent synthesis and indole-ring-analog generation. The Fischer indole synthesis would be perhaps one of the better suited methods for this purpose, and proved in fact highly effective in the synthesis of various monoterpenoid indole natural products. On the other hand, it was hardly exploited in the synthesis of Strychnos or uleine type alkaloids because their 2-azabicyclo[3.3.1]nonane ring ketone precursors are much less apt for the Fischer indolizations. Prompted by the synthetic limitations and potential merits of the Fischer indolization approach, we have devised new synthetic routes to (+)-uleine and (-)-tubifolidine via retro-Michael-Michel-triflation-indolization sequence. Our recent results in this line of chemistry will be presented.

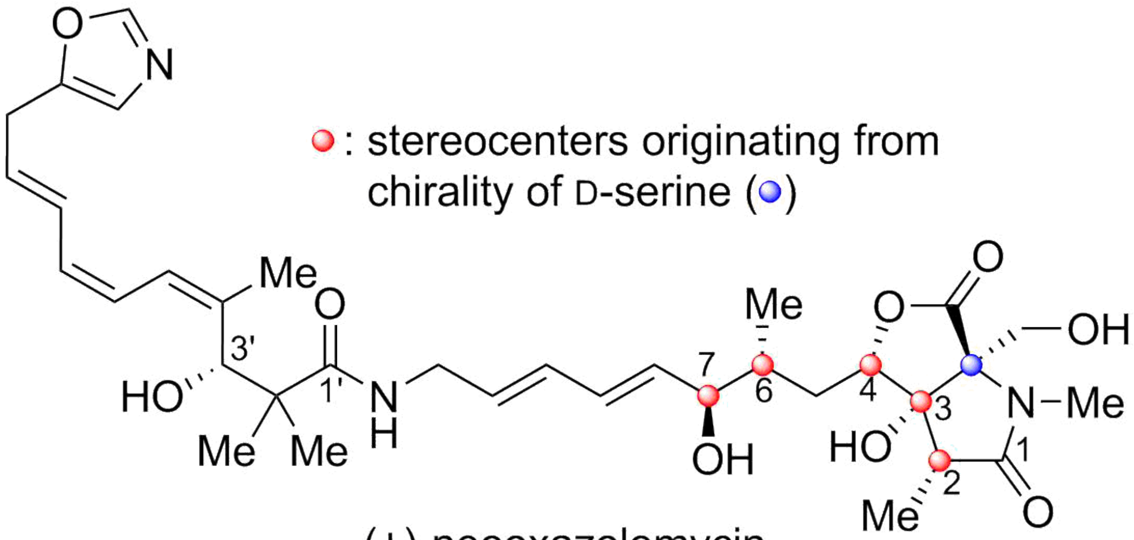
Symposium : **ORGN3-2**
Current Trends in Organic Chemistry II: Synthetic Methodology and Total Synthesis
Convention Hall 3, FRI 14:55
Chair: Kyungsoo Oh (Chung-Ang University)

Asymmetric Synthesis of Natural Products via Chirality Transfer Processes; Total Synthesis of (+)-Neooxazolomycin from D-Serine

Sanghee Kim

College of Pharmacy , Seoul National University, Korea

(+)-Neooxazolomycin, the first member of the oxazolomycin family of antibiotics, has been an attractive synthetic target. Oxazolomycins are characterized by a densely functionalized fused bicyclic system as well as a (Z,Z,E)-configured oxazole triene subunit. Considerable attention has been paid to the synthesis of this family of natural products because of their structural complexity and potent biological activities. However, there are only a few reports on their successful total syntheses.We achieved a biomimetic total synthesis of (+)-neooxazolomycin with a minimum number of chiral sources by a series of chirality transfer processes. In our synthesis, the six stereocenters in the right-hand fragment were established from D-serine as the only chiral source by chirality transfer processes including a ‘memory of chirality’ (MOC) and ‘dynamic kinetic resolution’ (DKR) assisted aldol reaction and substrate-controlled asymmetric inductions. The (Z,Z,E)-configured oxazole triene fragment was stereoselectively constructed, and the only chirality present in this fragment was installed by the asymmetric reduction of the ketone



(+)-neooxazolomycin

Symposium : **ORGN3-3**
Current Trends in Organic Chemistry II: Synthetic Methodology and Total Synthesis
Convention Hall 3, FRI 15:30
Chair: Kyungsoo Oh (Chung-Ang University)

Total Synthesis of (+)-Chamuvarinin and (-)-Jimenezin

Mallesham Samala, Thien Nhan Lu[1], Jongkook Lee[2,*]

Centre for marine natural products and drug, Indian Institute of Chemical Technology, India
[1]*Pharmacy, Ho Chi Minh City University of Technology , Vietnam*
[2]*College of Pharmacy, Kangwon National University, Korea*

Annonaceous acetogenins are a class of polyketides that bear tetrahydrofuran(s) (THF) and a terminal-lactone. Recent significant attention toward this class of natural products stems from their highly potent cytotoxicity against tumor cells by acting on mitochondrial complex I. It is believed that metformin also exhibits anti-cancer effects by targeting mitochondrial complex I. A number of clinical studies for combination therapy with metformin and other cancer drugs are undergoing. Chamuvarinin, the first reported annonaceous acetogenin bearing a tetrahydropyran (THP) ring adjacent to a bis-tetrahydrofuran (THF-THF) ring system, was isolated from the root of Uvaria chamae by Laurens and co-workers in 2004. Chamuvarinin possesses an adjacently linked oxatricyclic core with seven stereogenic centers along with a butenolide moiety with an eighth stereocenter. Chamuvarin showed strong anti-proliferative activity against KB3-1 (GI50 0.8 nM), a multi-drug resistant cervical cancer cell line. Jimenezin, an annonaceous acetogenin bearing a hydroxylated tetrahydropyran (THP) ring adjacent to a tetra-hydrofuran (THF) ring system, was isolated from the seeds of Rollinia mucosa (Jacquin) Baillon by Mata and co-workers in 1998. Jimenezin is constituted with an adjacently linked oxabicyclic core with six stereogenic centers and a butenolide moiety with an seventh stereocenter like chamuvarinin. Jimeneizin also displayed strong anti-cancer effects against several solid tumor cell lines. These challenging structural features and their unique biological activity have prompted us to seek efficient synthetic pathways to these targets. We herein present stereoselective synthetic approaches to (+)-chamuvarinin and (-)-Jimenezin, wherein their backbones were constructed in a substrate-controlled fashion by utilizing iterative chelation-controlled nucleophilic addition and internal alkylation.

Symposium : **ORGN3-4**

Current Trends in Organic Chemistry II: Synthetic Methodology and Total Synthesis

Convention Hall 3, FRI 15:55

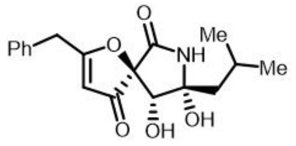
Chair: Kyungsoo Oh (Chung-Ang University)

Biosynthetically Inspired Synthesis of Complex Natural Products

Sunkyu Han

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

What are the modern roles and prospects of natural products synthesis? The rapid pace at which this world is changing makes this simple question non-trivial. Our laboratory undertakes natural products synthesis research with the following key words in mind: 1) Novel Strategy, 2) New Reactivity, and 3) Extraordinary functions of the target secondary metabolites. To be more specific, 1) Our group seeks to form multiple desired bonds in a single transformation and pursues synthetic strategies that involve drastic molecular backbone rearrangements. 2) We searches for aggressive bond disconnections that require the development of unprecedented synthetic methods involving novel reactivity. 3) We aim to devise practical synthetic solutions that can produce the natural products in sufficient quantity for further functional studies. Herein, syntheses of natural products that have been completed in our laboratory with these goals in mind will be presented.[1,2,3] References1 Kim, G.; Kim, M. J.; Chung, G.; Lee, H.-Y.; Han, S. *Org. Lett.* **2018**, *20*, 6886. 2 (a) Jo, D.; Han, S. *Org. Chem. Front.* **2017**, *4*, 506. (b) Kang, T.; Jo, D.; Han, S. *J. Org. Chem.* **2017**, *82*, 9335. (c) Jo, D.; Han, S. *Chem. Comm.* **2018**, *54*, 6750. (d) Jo, D.; Han, S. *Org. Lett.* **2019**, *21*, 6045.



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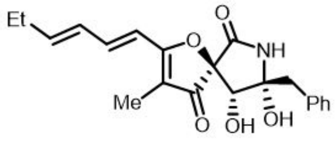
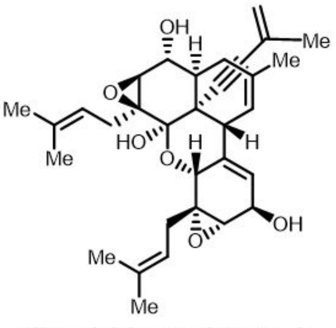


azaspirene



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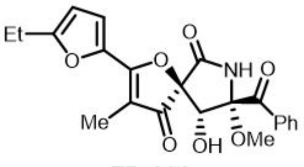

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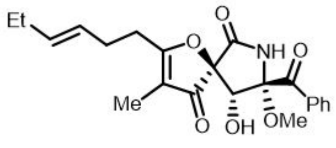


cephalimysin A

Symposium : **MEDI-1**
Innovative Therapeutics and Diagnostic Agents in Medicinal Chemistry
Room 606+607, THU 15:40
Chair: Hwan Jung Lim (KRICT)

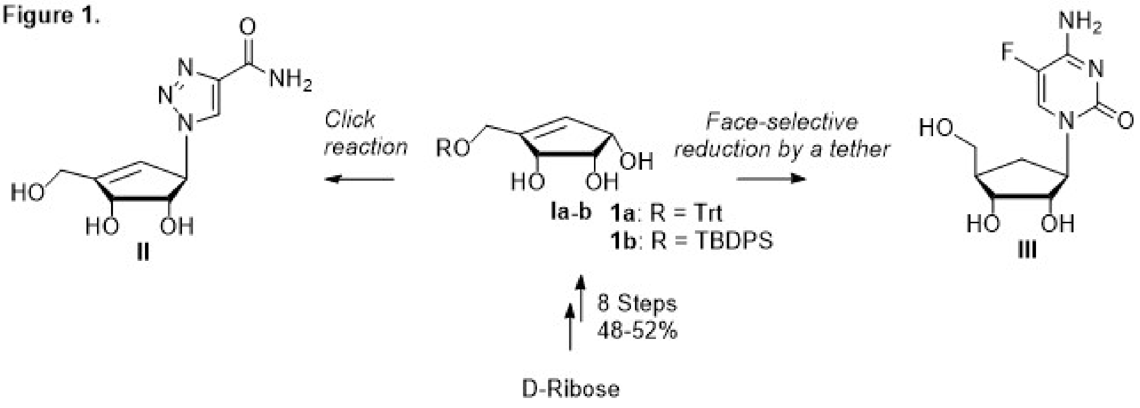
Practical Synthesis and Biological Evaluation of Carbocyclic Nucleoside Analogs

Jong Hyun Cho

Medicinal Biotechnology, Dong-A University, Korea

A practically synthetic method for chiral cyclopentenol derivatives (Ia-b) was developed as the key intermediate that was utilized for the synthesis of biologically active carocyclic nucleosides, From D-ribose, the selective protection of allylic hydroxyl group followed by the ring closing metathesis (RCM) reaction with Grubbs' catalyst II provided a single cyclopentanol (Ia) in 48-52% yield. The key intermediate was applied for the synthesis of unnatural five-membered ring heterocyclic carocyclic nucleosides as the neplanocin A (NPA). The novel structure, 1,2,3-triazolenucleoside (II), exhibited potent antiviral activity (EC50 0.4 μM) against vaccinia virus. In addition, the chiral cyclopentenol derivative (Ib) was used to develop an efficient synthetic route for biologically relevant (-)-5-fluorocarbodine (III), which is a potent anti-cancer agent. Direct coupling of N6-protected 5-fluorouracil with the cyclopentenol (1b), followed by formation of a macrocycle between the base and sugar moiety, via RCM reaction, allowed for a facial selective hydrogenation of the sugar double bond to give, exclusively, the desired 4'-β-stereoisomer (III).

Figure 1.



Symposium : **MEDI-2**
Innovative Therapeutics and Diagnostic Agents in Medicinal Chemistry
Room 606+607, THU 16:10
Chair: Hwan Jung Lim (KRICT)

Stimuli-responsive nano-therapeutics based on hyaluronic acid

Ki Young Choi[*], Jae Hyung Park[1]

Natural Product Informatics Research Center, Korea Institute of Science and Technology, Korea
[1]*Division of Chemical Engineering, Sungkyunkwan University, Korea*

Stimuli-responsive drug delivery nanomaterials have gained much attention as intelligent therapeutic means for the treatment of diverse diseases given that they can prolong bioavailability of chemo-/bio-therapeutic agents and enable activation of their therapeutic or diagnostic functions at the target disease tissues. By securing both blood stability and stimuli-responsive activation, it is possible to improve therapeutic efficacy while reducing adverse toxicity to the normal tissues. HA is a naturally occurring polysaccharide; it is highly water-soluble, biocompatible and biodegradable. HA also has unique biological traits such as strong binding with cell surface receptors such as CD44 and catabolism by HA-degrading-enzyme, hyaluronidases, ROS or RNS. Given the desired biological properties of HA, we have been employed HA as a building block or surface coating materials for targeted, stimuli-responsive drug delivery systems. In this talk, recent advances in designing stimuli-responsive HA nanomaterials that we developed will be reviewed and their diagnostic and therapeutic potential will be discussed.

Symposium : **MEDI-3**

Innovative Therapeutics and Diagnostic Agents in Medicinal Chemistry

Room 606+607, THU 16:50

Chair: Jungwook Chin (DGMIF)

Synthesis and Optimization of 4-Aryl-*N*-(2-alkoxythieno[2,3-*b*]pyrazine-3-yl)-4-arylpiperazine-1-carboxamide Derivatives as an Anti-colorectal Treatment toward a Novel FBW7 Selective Drug Target

Young Dae Gong

Department of Chemistry, Dongguk University, Korea

Cancer cells are characterized by an abnormal cell cycle. Many anticancer agents targeting proteins involved in cell cycle control have been developed. We have developed a new lead compounds, core skeleton of 2-alkoxythieno[2,3-*b*]pyrazine-3-yl)-4-arylpiperazine-1-carboxamides via DGG-200064 (**64**). The new series of lead compound synthesized were shown to regulate colorectal cancer cell that induces G2/M arrest in colorectal cancer cells. The **64** (GI_{50} = 25 nM in a HCT116 cell-based assay), unlike the known cell cycle inhibitors, has been shown to inhibit the interaction of FBW7 and c-Jun, resulting in G2/M arrest. To prove and develop a leading compound, the lead compounds evaluated *in vivo* colorectal cancer xenograft models using HCT116 and Colo205 cells in rats. The *in vivo* growth inhibition were showed high efficacy and their PK properties were also evaluated in rats. From the results of lead compound **64** was suggested for the further development as an orally deliverable anti-colorectal cancer drug as a novel drug target.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Symposium : **MEDI-4**
Innovative Therapeutics and Diagnostic Agents in Medicinal Chemistry
Room 606+607, THU 17:20
Chair: Jungwook Chin (DGMIF)

Discovery of FB-101, a novel clinical candidate for the treatment of Parkinson’s disease

Jinhwa Lee

1ST Biotherapeutics lnc, Korea

Parkinson’s disease is a progressive neurodegenerative disease characterized by loss of dopaminergic neurons in the substantia nigra. Aggregation of alpha-synuclein contributes to the formation of Lewy bodies and neurites, the pathologic hallmarks of alpha-synucleinopathies such as Parkinson’s disease (AD), dementia with Lewy bodies (DLB), and multiple system atropy (MSA). An increase in c-abl activity via phosphorylation has been reported to be associated with alpha-synuclein pathology detected in Parkinson disease and other neurodegenerative disease. Recently, administration of nilotinib, a c-abl inhibitor, in a small pilot clinical trial on PD and DLB patients showed potential therapeutic option of c-abl inhibition for PD therapy. However, nilotinib has moderate brain penetration in mice and human, not enough to show optimal efficacy for CNS manifestation. In addition, nilotinib has a safety issue, not suitable for usage in chronic neurodegenerative disease. Therefore, a c-abl inhibitor with better properties, improved brain penetration, and bigger therapeutic window than nilotinib will position as a disease modifying agent for novel PD therapeutics. Along the line, we will discuss the discovery of FB-101, a novel clinical candidate for the treatment of Parkinson’s disease, showing its strong competitive position over nilotinib and other related TKI competitors. We have discovered FB-101, a novel clinical candidate for treatment of Parkinson’ disease with potential to expand into other neurodegenerative diseases. FB-101 is a 1STBIO’s proprietary molecule with strong efficacy, supreme selectivity, and CNS-drug likeness which we expect to be successfully translated into clinical efficacy as a novel disease-modifying agent for Parkinson’s disease.

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

Special Symposium on the Present and Future of Materials Chemistry

Room 700B, THU 17:20

Chair: Hyeon Suk Shin (UNIST)

Entropy driven strategy to harness entire solar spectrum

Doo-Hyun Ko

Department of Applied Chemistry, Kyung Hee University, Korea

The conversion and manipulation of light via lanthanide-based upconversion (UC) and downshifting (DS) show promise in numerous applications. We demonstrate the lanthanide-doped nanotemplates to improve conversion of ultraviolet and near-infrared to visible light through resonant-mode excitation. The templates are fabricated using nanoimprint technique wherein ordered arrays of nanoscale features are readily made over large areas. The practical applicability of this platform in photovoltaic devices is evaluated, showing distinctively enhanced efficiency. The material-agnostic nanopatterning methodology is further extended to nanopatterned thin films synthesized by a sol-gel-based solution to achieve simultaneous photonic and electrical enhancements in thin film photovoltaic devices. For further approach, we demonstrate the use of quaternary bulk heterojunctions composed of two conjugated polymer donors and two fullerene acceptors as a novel platform to produce high-efficiency and long-term durable organic photovoltaics. We attribute the enhanced stability to the significant suppression of domain growth and phase separation between the components via kinetic trapping effect.

Symposium : **MAT1-1**
Special Symposium on the Present and Future of Materials Chemistry
Room 700B, THU 15:40
Chair: Hyeon Suk Shin (UNIST)

Crystallographic approach to design of new fast lithium-ion conductor

Jaegyeom Kim, Doe-hee Park, Minseong Kim, Gunwoo Yoo, Seung-Joo Kim*

Department of Energy Systems Research, Ajou University, Korea

The lithium-ion conducting oxides have attracted world-wide attention due to the possible application as a solid electrolyte. Generally, fast lithium-ion conducting oxides have framework structures composed of corner-sharing metal-centered octahedra ($MO_{6/2}$) and tetrahedra ($TO_{4/2}$), which are represented by a general formula $A_x(MO_{6/2})_m(TO_{4/2})_n$. We recently prepared a new lithium-ion conducting oxide, $LiTa_2PO_8$, corresponding to the composition with $m = 2$ and $n = 1$, *i.e.*, $Li(TaO_{6/2})_2(PO_{4/2})$. The synchrotron X-ray/neutron powder diffraction analysis revealed that that the TaO_6 octahedra and PO_4 tetrahedra are connected via corner-sharing to form an unprecedented anionic framework providing an effective 3*D* pathway for lithium-ion conduction. The sintered $LiTa_2PO_8$ pellets exhibited an excellent lithium-ion conductivity (2.5×10^{-4} S cm^{-1} at 25 °C), which are comparable or superior to the highest values reported to date for other fast ion conductors such as perovskite $Li_{3x}La_{2/3-x}TiO_3$, NASICON $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$, and garnet $Li_7La_3Zr_2O_{12}$. In this presentation, we classify various lithium-containing oxides with framework structure according to the ratio of octahedral and tetrahedral units, and then we predict possible migration pathways of lithium ions in each lattice based on simple Bond Valence Sum calculations. This approach would be useful for designing new materials with improved lithium conductivity.

Symposium : **MAT1-2**

Special Symposium on the Present and Future of Materials Chemistry

Room 700B, THU 16:05

Chair: Hyeon Suk Shin (UNIST)

Designing Nanostructured Catalytic Materials for Promoting Renewable Energy Conversion Reactions

Sang Hoon Joo

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

“Hydrogen economy” is considered as a long-term solution for securing our energy future. A kry element for realizing this compelling vision is the development of highly active, durable, and low-cost electrocatalysts for energy conversion reactions, such as fuel cells and electrolyzers. Our group has designed and prepared new electrocatalysts for oxygen reduction reaction, H_2O_2 production, oxygen evolution reaction, chlorine evolution reaction, and hydrogen evolution reaction through the understanding of active sites for enhancing their activity, selectivity, and durability. In this talk, I will present our recent efforts toward designing nanostructured electrocatalysts based on low-precious metal, non-precious metal, and carbon-based compositions. I also present our endeavor for identifying catalytically active sites in these electrocatalysts by in situ spectroscopic and computational methods, and applying the developed electrocatalysts in system-level devices.

Symposium : **MAT1-3**

Special Symposium on the Present and Future of Materials Chemistry

Room 700B, THU 16:30

Chair: Hyeon Suk Shin (UNIST)

Future Directions with Complex Nanoparticles with Tailored Functions: Manipulation of Localized Surface Plasmon Resonance (LSPR)

Sungho Park

Department of Chemistry, Sungkyunkwan University, Korea

The paper represents a new approach for a dynamic three-dimensional (3-D) sensing platform based on stochastics from the collective behaviour of active magnetic-plasmonic nanorods; this approach utilizes shear-force induction under an external magnetic field in contrast to a traditional LSPR-based biosensing platform that is operated in passive and stationary conditions, limiting any additional modulation of the detection system. Au/Fe/Au nanorods exhibited plasmonically-active behaviour through plasmonic coupling, and the middle ferromagnetic Fe block responded to a magnetic impetus, enabling the nanorods to be modulated. Rotation of the magnetically-active nanorods produces periodic wave signals due to the intrinsic optical anisotropy of the nanorods, which can be analysed by converting the time domain into the frequency domain using the fast Fourier Transform method. Importantly, by introducing specific binding events, a dynamically-perturbed system was realized, resulting in the phase lag of nanorods above a critical driving frequency. As a proof-of-concept, we applied this system to detect influenza virus (HA1) with a shear force-induced rotating platform. We were able to achieve a limit of detection (LOD) that was two orders of magnitude lower than that of an analogous conventional LSPR sensing setup. Additionally, we will briefly discuss about the possible multi-step synthetic strategy leading to the complex nanoparticles with which the localized surface plasmon resonance can be further modulated for full harvesting the near-field electromagnetic field.

Symposium : **MAT1-4**
Special Symposium on the Present and Future of Materials Chemistry
Room 700B, THU 16:55
Chair: Hyeon Suk Shin (UNIST)

Dynamic Nanostructures through Self-Assembly of Functional Polymers and Nanoparticles

So-Jung Park

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

Here, we present new approaches for the fabrication of stimuli-responsive dynamic nanostructures. Dual-responsive DNA diblock copolymers and triblock copolymers were synthesized by coupling a thermo-responsive polymer, poly(N-isopropylacrylamide (PNIPAM) and an oligonucleotide. Such DNA block copolymer micelles can undergo sphere-to-cylinder shape transformation in response to the temperature change and programmable DNA binding events, demonstrating the multi-dimensional dual responsive shape changing capability. Furthermore, we present a new approach to fabricate dynamic and responsive free standing films of nanoparticles, based on the programmable DNA-directed self-assembly and the layer-by-layer (LbL) thin film fabrication technique. We demonstrate that the new approach provides a powerful means to generate dynamic nanostructures that can undergo complex and programmable shape transformation.

Symposium : **MAT2-1**
Current Trends in Quantum Dots: Synthesis and Application
Room 700B, FRI 09:00
Chair: Jongnam Park (UNIST)

Designed synthesis of colloidal nanocrystals and their optoelectronic applications

Jiwoong Yang

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

Fundamental understanding on the nanocrystal formation process is essential to fully exploit their unique properties for various applications. However, their formation mechanism is known to be very difficult to study. Herein, I will present my research on the nanocrystal formation and their optoelectronic applications. I will talk about the prenucleation magic-sized clusters, important intermediate species for nanocrystal synthesis. I will discuss the research on the nanocrystal formation process using in-situ liquid phase transmission electron microscopy. Furthermore, I will present the application of quantum dots for optoelectronic applications (e.g., solar cells and light-emitting diodes).

Symposium : **MAT2-2**

Current Trends in Quantum Dots: Synthesis and Application

Room 700B, FRI 09:30

Chair: Jongnam Park (UNIST)

Surface Chemistry and Engineering of Colloidal Semiconductor Nanocrystals for Photovoltaic Applications

Younghoon Kim

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

Colloidal semiconductor nanocrystals have been attracted considerable attention in various optoelectronic applications such as solar cells, light-emitting diodes, etc. Owing to their size-, composition-tunable optical bandgaps, excellent photophysical properties, and low temperature solution processibility. In this presentation, we present the photovoltaic device applications based on colloidal quantum dot nanocrystals. Colloidal quantum dot nanocrystals are synthesized via hot-injection methods using long-chain insulating ligands (i.e., oleic acid, oleylamine, etc.). The original ligands of as-synthesized colloidal quantum dots should be replaced with organic/inorganic short chain ligands in order to enhance the charge transporting within the nanocrystal-based thin films. We also should consider optimum ligands, surface passivation, final film thickness as well as device architectures for further improved photovoltaic performance. Considering all the properties above-mentioned, we here demonstrate the perspective and recent research trend of colloidal quantum dot-based photovoltaic applications.

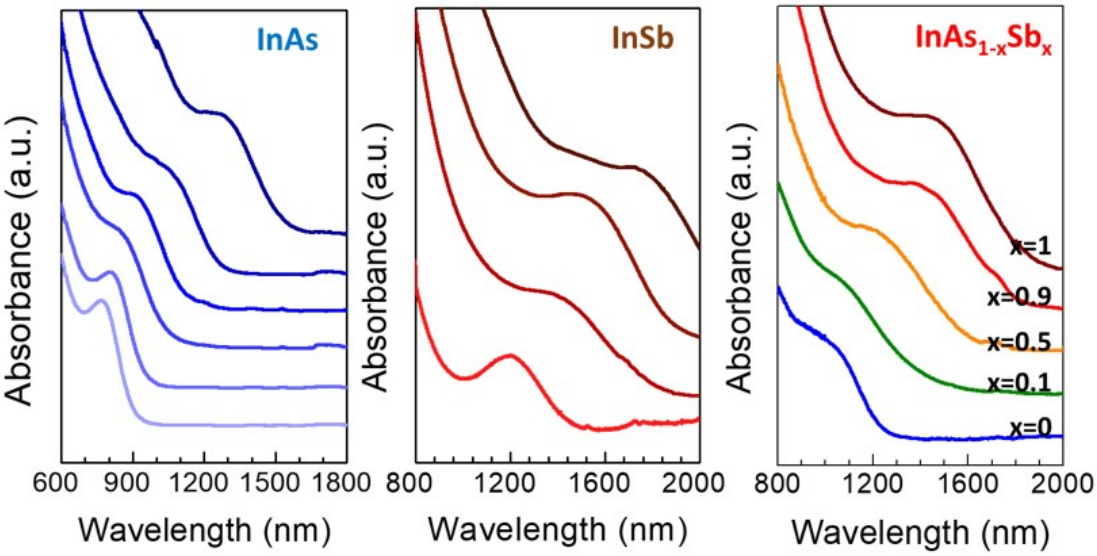
Symposium : **MAT2-3**
Current Trends in Quantum Dots: Synthesis and Application
Room 700B, FRI 10:00
Chair: Jongnam Park (UNIST)

General Synthetic Route to High Quality Colloidal III-V Semiconductor Quantum Dots

Nuri Oh

Division of Materials Science and Engineering, Hanyang University, Korea

The synthesis of colloidal III-V quantum dots (QDs), particularly of the arsenides and antimonides, has been limited by the lack of stable and available group V precursors. In this work, we exploit InCl3 and pnictogen precursors to synthesize III-V QDs. Through co-reduction reactions of the precursors, we achieve size and stoichiometry-tunable, binary InAs and InSb as well as ternary alloy InAs1-xSbx QDs (Figure). Based on structural, analytical, optical, and electrical characterization of the QDs and their thin-film assemblies, we study the effects of alloying on their particle formation and optoelectronic properties. We introduce a hydrazine-free hybrid ligand exchange process to improve carrier transport in III-V QD thin films and realize InAs QD field-effect transistors with electron mobility >5 cm2/Vs. We demonstrate that III-V QD thin films are promising candidate materials for infrared devices and show InAs1-xSbx QD photoconductors with superior short-wavelength infrared (SWIR) photoresponse than those of the binary QD devices.


InAs
InSb
$InAs_{1-x}Sb_x$
Absorbance (a.u.)
Absorbance (a.u.)
Absorbance (a.u.)
600
900
1200
1500
1800
800
1200
1600
2000
800
1200
1600
2000
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
x=1
x=0.9
x=0.5
x=0.1
x=0

Symposium : **MAT2-4**
Current Trends in Quantum Dots: Synthesis and Application
Room 700B, FRI 10:30
Chair: Jongnam Park (UNIST)

Colloidal II-VI Semiconductor Nanorods: Growth and Assembly Controlled by Surface Ligands

Doh Chang Lee

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

Growth of monodisperse quantum dots (QDs) is a pressing requirement in the context of commercial application as well as academic study, as the size uniformity is directly related to color purity in display products which have been commercialized. In the sense, understanding on the generation of active species via thermolysis of precursors, diffusion of precursors from bulk solution onto nanocrystal surface, and surface growth reaction kinetics has been ever more important. In this presentation, I will present our recent findings pertaining to these issues on the basis of different material examples. We have investigated diffusion of active species monomers through ligand layers using CdSe nanorods (NRs) as a model system. Colloidal NRs are of special interest for optoelectronic applications because its shape anisotropy leads to unique optical and physical characteristics, expandable with morphological and structural deviation. Previous studies focused on the development of diverse NR structures. However, synthesis relied on empirical observations under specific conditions, and general NR growth process remained elusive. I present a new answer for detailed growth mechanism of colloidal semiconductor NRs. For this, we developed dual-diameter nanorod (DDNR) structure via colloidal synthesis, where two sections along the long axis in each NR have different diameters at a few nanometer scale. The vivid segmentation is an ideal platform for monitoring the growth process of NRs, presenting important determinants in the reactivity of distinguishable NR facets. The lesson obtained from DDNR is universally applied to nanocrystal growth in any colloidal batch. By controlling the discovered factors, single-diameter NRs with controllable core position also became available. I will put the findings in perspective by outlining the effect of diffusion of monomers and surface growth reactions.

Symposium : **MAT3-1**

Understanding Materials and Device Aspects of Hybrid Light-emitters

Room 700B, FRI 14:30

Chair: Jaemin Lee (KRICT)

Probing molecule-like isolated octahedra: Phase stabilization of zero-dimensional cesium lead halide QD

Won Bin Im

Division of Materials Science and Engineering, Hanyang University, Korea

Zero-dimensional (0D) inorganic perovskites have recently emerged as a new class of material for optoelectronics owing to their outstanding excitonic properties, strong photoluminescence (PL), and high exciton binding energy. These materials have a unique quantum-confined structure, which originates from the presence of fully isolated octahedra exhibiting single-molecule behavior. In this work, we probed the optical behavior of single molecule-like isolated octahedra in 0D Cs_4PbX_6 (X = Cl, Br/Cl) perovskite through isovalent (Mn^{2+}) doping at Pb sites. The incorporation of Mn^{2+} stabilizes the Cs_4PbX_6 phase by lowering the symmetry of PbX_6 via enhanced octahedral distortion (preventing the high-symmetry cubic $CsPbX_3$ impurity) and controlling the compositional variation of Cs-Pb salts. This strategy enabled the synthesis of $CsPbX_3$ free Cs_4PbX_6 nanocrystals. A high PL quantum yield (QY) of Mn^{2+} emission was obtained in the colloidal (29%) and solid (21%, powder) forms. These performances can be attributed to structure-induced confinement effects, which enhance the energy transfer from localized host exciton states to Mn^{2+} dopant within the isolated octahedra of 0D perovskite. The present findings could lead to designing of low-dimensional perovskites as efficient light emitters with photo and chemical stability for high-performance optoelectronic devices.

Symposium : **MAT3-2**
Understanding Materials and Device Aspects of Hybrid Light-emitters
Room 700B, FRI 15:00
Chair: Jaemin Lee (KRICT)

Highly Efficient Perovskite Light-Emitting Diodes by Surface Engineering and Defect Passivation

Myoung Hoon Song

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

The organic-inorganic hybrid perovskite materials have been interested because of their outstanding electrical and optical characteristics, which enables a remarkable enhancement of device efficiency. However, high-quality perovskite nanocrystal films are required to realize highly efficient and stable perovskite LEDs. Here, we demonstrate the current strategies involved in the morphological control of perovskite films to improve the device performance and long-term stability of PeLEDs via perovskite film modification, interface engineering, and self-organized multiple quantum wells (quasi 2D-perovskite).

Symposium : **MAT3-3**
Understanding Materials and Device Aspects of Hybrid Light-emitters
Room 700B, FRI 15:30
Chair: Jaemin Lee (KRICT)

Reversible, full color luminescence by post-treatment of perovskite nanocrystals

Gihwan Kim

Photonics Energy Research Center, Korea Photonics Institute Technology(KOPTI), Korea

Organometal halide (Cl, Br, I) perovskite is one of the best candidate materials for the next generation of opto-electronic devices, such as solar cells and LEDs, due to its high performance and low cost. Synthesis of nanocrystals based on halide perovskites is a convenient way to make perovskite with targeted halide ratio and band gap. Interestingly, halides in perovskite have some freedom in crystal to be exchanged with other halides even in ligand-capped nanocrystals. Therefore, post-treatment can be used to control the halide ratio in nanocrystals to achieve a finely controlled desired band gap of perovskite nanocrystal. In this research, halide anions in synthesized halide perovskite nanocrystals are finely controlled after synthesis via commonly used haloalkane solvents and nucleophiles. This post-treatment by adjusting the anion halides in perovskite materials can be widely applied to various purposes and applications such as LEDs and solar cells. A fully reversible (CsPbCl3 ⇌ CsPbBr3 ⇌ CsPbI3) post-treatment method of anion exchange for CsPbX3 (X = Cl, Br, I) perovskite nanocrystals conducted with haloalkane solvent and nucleophile is presented. Through the control of anion-exchange kinetics, the band gaps of nanocrystals are finely tuned covering the full wavelength region from 400 to 700 nm. The dissociation mechanism of haloalkane solvent with nucleophile is clearly explained with SN2 chemical reaction to produce halide anions. With the post-treatment method, fabricated LED devices showed highly saturated RGB colors.

Symposium : **MAT3-4**

Understanding Materials and Device Aspects of Hybrid Light-emitters

Room 700B, FRI 16:00

Chair: Jaemin Lee (KRICT)

Optical-electrical characterization of multidimensional perovskite and its applications

Jin Woo Choi

Korea Institute of Materials Science, Korea

Organometallic halide perovskite has attracted attention due to its outstanding and optimistic energy conversion efficiency in photovoltaic field. Recently, Organic-inorganic lead halide perovskite is emerging as a potential emissive material for light emitting devices such as light emitting diodes (LEDs) and lasers, which has emphasized on the necessity of understanding its fundamental opto-physical properties.Temperature-dependent photoluminescence of CH3NH3PbBr3 perovskite quantum dots (QDs), polycrystalline thin film (TF) and single crystal (SC) have been studied. The opto-physical properties such as exciton-phonon scattering, exciton binding energy and exciton decay dynamics, were investigated. The studies revealed that the primary non-radiative exciton decay pathway for QDs is the phonon assisted thermal escape while that for TF and SC was the thermal dissociation due to low exciton binding energy. Base on this knowledge, multidimensional perovskites were introduced to various applications.

Symposium : **ELEC1-1**
In operando? Emerging Techniques for Electrocatalysis
Room 603+604, THU 15:40
Chair: Sang-Il Choi (Kyungpook National University)

Photoelectrochemical CO2 Reduction into Liquid Products: Multi-electron Shuttling, Reduction Potential Tuning and CO2 Activation

Young Soo Kang

Department of Chemistry, Sogang University, Korea

CO2 reduction driven by(040)-facet engineered BiVO4 plate photoanode(040)-BVO) is investigated for solar fuel production. In the photoelectrochemical CO2 reduction reaction, water oxidation reaction is performed on (040)-BVO and chemical fuels is obtained on Cu cathode in the CO2-saturated NaCl electrolyte under AM 1.5 G. C1 chemical fuel is evolved through reduction potential depending multistep process from CO2 molecule. 040-BVO(photoanode)/NaCl(electrolyte)/Cu(cathode) system is illuminated with solar light under the external bias that is tailored to reduce CO2 via reduction potential tuning. Integrating applied bias potential into conduction band minimum of 040-BVO enables CO2 molecules to be converted into valuable chemical fuels. This thermodynamic control leads to the product selectivity and an increase in the faradaic efficiency. We observe that the selectivity and yield of the products depend on CO2 reduction potential tuning. With water oxidation reaction of 040-BVO photoanode which has 42.1% of the absorbed photon-to-current conversion efficiency at 1.23 V (vs RHE), chemical products were observed as faradaic efficiency of 30% formic acid, 60% formaldehyde, 12% MeOH and 3% EtOH by reduction potential tuning. For this study, the correlation between the production of solar chemical fuels and CO2 reduction potential tuning via external bias potential on 040-BVO photoanode/Cu photocathode is systematically investigated, and we suggest that the results of this study represent the most viable strategy.

Symposium : **ELEC1-2**
In operando? Emerging Techniques for Electrocatalysis
Room 603+604, THU 16:10
Chair: Sang-Il Choi (Kyungpook National University)

Operando characterizations for fundamental understandings of electrochemical reactions in the nitrogen-cycle

Chang Hyuck Choi

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

In nature, conversion of nitrogen species is controlled by enzymatic reactions, called the nitrogen cycle. However, excessive amounts of NO_x and other forms of nitrogen species from the industry have induced severe environmental problems. Therefore, it is well worth considering energy conversions from nitrogen-based pollutants to N_2 or hydrogen carrier (e.g. NH_3 and NH_2OH) by artificial nitrogen-cycle catalysis. In that sense, NH_3 is one of the promising candidates to store hydrogen and energy efficiently, which has high hydrogen content and capability of liquefaction. Although the platinum has been known as the best electrocatalyst for the NH_3 oxidation reaction, its successful introduction into the industry suffers from the poor stability of the platinum. We study the deactivation mechanism with NO_x-modified platinum and show the detrimental roles of the NO_x species towards the NH_3 oxidation reaction. In the opposite strategy, NO_x reduction to N_2 or NH_3 has also attracted attention for reducing pollutants and hydrogen carrier synthesis. Since NO is known as a key intermediate in the NO_x reduction process, NO reduction is important to control reaction selectivity into N_2 or other valuable products (e.g. NH_3 and NH_2OH). We found that atomically dispersed iron-doped nitrogen-carbon catalysts (Fe-N-C) have >90 % selectivity to NH_2OH, which has a low energy barrier to produce H_2 and an advantage on transport via a liquid phase. This study proposes that the selectivity control may be achieved by designing the ensemble structure.

Symposium : **ELEC1-3**
In operando? Emerging Techniques for Electrocatalysis
Room 603+604, THU 16:35
Chair: Sang-Il Choi (Kyungpook National University)

Understanding electrocatalytic carbon dioxide conversion

Youngkook Kwon

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

The efficient electrochemical conversion of CO2 to fuels or stock chemicals with high-energy density would be a major step forward in the introduction of a carbon neutral energy cycle, as it would allow for the direct low-temperature conversion of photo-generated electrical current to stored chemical energy, in a manner very similar to the way nature stores solar energy. The high activity and selectivity towards electrocatalytic conversion of CO2 can be achieved with careful selection of catalyst and electrolyte. Especially, understanding the role of electrocatalysts and electrolytes that can efficiently reduce CO2 to fuels with high selectivity is a subject of significant interest. In this talk, I'll introduce diverse in-situ techniques to unravel the reaction mechanism for efficient electrochemical CO2 conversion.

Symposium : **ELEC1-4**
In operando? Emerging Techniques for Electrocatalysis
Room 603+604, THU 17:00
Chair: Sang-Il Choi (Kyungpook National University)

In- and ex-situ TEM for battery materials

Jong Min Yuk

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

Rechargeable batteries receive intensive research effort, with a wide range of application space including mobile electronic devices, electric vehicles and grid-scale energy storage. The limit in battery capacity partly arises from our lack of understanding on the crystal structure and morphology evolution of the electrode materials during operation. In this talk, we show in-situ transmission electron microscopy techniques that investigate this missing link with unprecedented temporal and spatial resolution. The first example studies the sodiation pathways of graphene-coated copper sulfide particles. In particular, we reveal sequential phase transition pathways that deviate from the thermodynamic equilibrium and the semi-coherent phase boundaries during the conversion reaction. We rationalize that this unique interface behavior alleviates the particle pulverization during cycling and thus explains the high reversible capacity without excessive morphology optimization. In the second example, we show stress-driven composition change in core-shell SnO_2-Sn nanoparticles. Especially, the generation of non-uniform composition field is directly visualized with in-situ graphene liquid cell electron microscopy. These in-situ observations explore the nanoscale regime previously unaccessible with conventional characterization tools and provide scientific insights on the microstructural and phase evolution during alkali ion insertion, a technologically relevant field in energy storage and energy harvester systems.

Award Lecture in Division : **ELEC2-4**

Recent Progress in Photoelectrochemistry

Room 603+604, FRI 10:30

Chair: Soon Hyung Kang (Chonnam National University)

Fundamental Understanding of Electrochemical Phenomena Enables the Development of Processes and Products

Woonsup Shin

Department of Chemistry, BioMedical Engineering, Sogang University, CareMedi, Co., Korea

Electrochemistry is a discipline of science and technology connecting electron transfer reactions with electrical input and output through electrodes. Therefore, electrochemistry has fundamentally multidisciplinary nature which relates to chemistry, chemical engineering, material science, process engineering, electronics and electrical engineering, etc. The key element in electrochemistry is the electrode where electrochemical reaction, reduction or oxidation, occurs. The understanding of electrode materials and electrochemical process is the most important in developing the devices and the processes, which can be applied to the fields of energy conversion, power sources, environmental processes, medical devices and sensors. In this talk, the correlation of the fundamental understanding of the electrode materials and the electrochemical processes with the actual applications in carbon dioxide conversion and medical device development in drug delivery and sensors will be focused.

Symposium : **ELEC2-1**

Recent Progress in Photoelectrochemistry

Room 603+604, FRI 09:00

Chair: Soon Hyung Kang (Chonnam National University)

Efficient Solar Water Oxidation over Perovskite-type Oxynitride Photoanodes

Jeongsuk Seo

Research Initiative for Supra-Materials (RISM), Shinshu University, Japan, Korea

The n-type visible-light-responsive (oxy)nitrides such as Ta3N5 and perovskite-type oxynitrides having a formula AB(O,N)3 (A=Ca, Sr, Ba and La, B=Ti, Ta and Nb) are capable of absorbing a wide wavelength range of visible light (band-gap energy, Eg; 1.7~2.1 eV). Band edge potentials of the (oxy)nitrides straddle water redox potentials so that these materials drive solar-driven overall water splitting thermodynamically. Based on the favourable optical property, a Ta3N5 photoanode has already presented significant improvement reaching to theoretical maximum photocurrent density of 13 mA cm-2 at 1.23 VRHE toward the water splitting. However, the long-term photoactivity is still low and the onset potential for anodic photocurrent density is highly positive. Also, the presence of B species in AB(O,N)3, which are readily reduced during nitridation because of the high electronegativity of B, promotes the generation of defects and/or impurities at oxynitride surface.The photovoltage generated by an oxynitride in response to irradiation is typically low due to its narrow Eg. Thus, driving a water splitting over the oxynitride is significantly challenging. As such, physical properties of the oxynitride itself, such as low crystallinity of material and generation of surface defects during nitridation which enhance the recombination of photoexcited holes and electrons, become very critical for driving the photoreaction in conjunction with a small driving force. Herein I present recent advances in the water splitting activity over BaBO2N (B=Nb, Ta) photoanodes and a key issue for effective syntheses of oxynitrides to increase the degree of crystallinity and as well to suppress the generation of surface defects.

Symposium : **ELEC2-2**
Recent Progress in Photoelectrochemistry
Room 603+604, FRI 09:30
Chair: Soon Hyung Kang (Chonnam National University)

Photosynthesis of C1-C6 aliphatic acids using mixed oxide films with efficiency exceeding the photosynthesis limit

Hyunwoong Park

School of Energy Engineering, Kyungpook National University, Korea

The photocatalytic conversion of CO2 and water into value-added chemicals remains a great challenge. Most photocatalysts and their systems suffer from poor efficiency, mixed products, and short durability, while requiring auxiliary chemicals and electrical energy. However, uniformly mixed copper and iron oxide (CuO/CuFeO2; CFO) bulky heterojunction films are capable of converting CO2 and water at circum-neutral pH into C1-C6 aliphatic acid anions and O2 at a solar-to-chemical energy conversion (STC) efficiency close to 3% under simulated sunlight (AM 1.5; 100 mW cm-2) in the absence of any sacrificial chemicals or electrical biases. When the CFO film is simply wired to a Pt foil, C1 (formate) and O2 are produced at a near stoichiometric ratio at an STC efficiency of ~5%. The CFO films are durable over a week and recyclable over five weeks under continuous irradiation. The addition of chloride significantly enhances formate production, with an STC efficiency of 10%, while inhibiting the deformation of CFOs. Density functional theory computations support the observed selectivity and durability. A simple synthetic procedure, high efficiency close to that of photosynthesis, durability, recyclability, and earth-abundant compositions of CFO films meet most requirements for artificial photosynthesis.

Symposium : **ELEC2-3**

Recent Progress in Photoelectrochemistry

Room 603+604, FRI 10:00

Chair: Soon Hyung Kang (Chonnam National University)

Rational Design of Metal Oxide Based Nanostructures for Enhancing Photoelectrochemical Water Oxidation with Efficient Light Harvesting, Charge Separation, and Charge Transfer

Jung Kyu Kim

School of Chemical Engineering, Sungkyunkwan University, Korea

Photoelectrochemical (PEC) water splitting to produce hydrogen fuel is an attractive strategy to achieve a sustainable energy supply. To achieve stable hydrogen production, light harvesting, charge separation/transport, charge transfer, and the stability or durability of PEC cells are strongly required. In recent years, cost-effective, stable, and earth abundant n-type metal oxides have been extensively studied for the efficient PEC water oxidation. However, the slow charge migration, electronic-state-mediated rapid trapping, and poor surface catalytic kinetics of metal oxides remain a significant obstacle for its use as a water oxidation catalyst. As a part of our effort to achieve simultaneously high light absorption, charge separation, and charge transfer efficiencies, divergent metal oxide based photoanodes have been rationally designed to have efficient heterojunction structures. Our recent findings on strategies to improve the metal oxide nanostructure based photoelectrochemical water oxidation will be introduced in this talk.

Symposium : **EDU1-1**

Current Issues and Research in Chemistry Education

Room 605, FRI 09:00

Chair: JiHun Park (Busan Science High Schoool)

Current Status and Issues of IB Curriculum in the Future of Chemistry Education

Jongseok Park

Department of Chemistry Education, Kyungpook National University, Korea

International Baccalaureate's mission is “The International Baccalaureate aims to develop inquiring, knowledgeable and caring young people who help to create a better and more peaceful world through intercultural understanding and respect. To this end the organization works with schools, governments and international organizations to develop challenging programmes of international education and rigorous assessment. These programmes encourage students across the world to become active, compassionate and lifelong learners who understand that other people, with their differences, can also be right.”Recently, several local governments have attempted to introduce IB programs into school settings. In this regard, I consider the following question.What is IB? What is the science in the IB program and IB program? Is the IB program appropriate for Korea's science education environment?

Symposium : **EDU1-2**
Current Issues and Research in Chemistry Education
Room 605, FRI 09:40
Chair: JiHun Park (Busan Science High Schoool)

Learner's reflection and intellectual humility in higher education.

Chang-Hoon Nam

Daegu Gyeongbuk Institute of Science & Technology, Korea

First of all, I will discuss how learner's reflection in education is important. In the process of education, learner's reflection is essential from the point of discovering why learners themselves learn and to lead them to think about how their learning will be used in society.And I will discuss on the intellectual humility in higher education. We should think about ‘the nature of science’ before applying the abstract terminology of intellectual humility to discussions related to science education. Science is the foundation of ideas that make the world including human beings understandable. On the other hand, humans struggle to change the conditions of life based on what they understand. The world is too big and complicated for the individuals to look at their knowledge alone. We have to have a broader perspective and collaborate with others to recognise and properly respond to the world. In this way, the science in modern society is the base of worldview, the issue of education, and the question of morality.

Symposium : **EDU1-3**
Current Issues and Research in Chemistry Education
Room 605, FRI 10:20
Chair: JiHun Park (Busan Science High Schoool)

Impacts of Argument-based Modeling(AbM) strategy on the peer assessment and self assessment in high school science

Hyesook Cho, Eugene Kang[1], Jeonghee Nam*

Department of Chemical Education, Pusan National University, Korea
[1]*Pusan National University, Korea*

The purpose of this study was to investigate the impacts of Argument-based Modeling(AbM) strategy applying peer-assessment and self-assessment on science subject on modeling ability in high school students' summary writing. For this study, coeducational high school 2nd grade four classes(113 students) were selected two class were assigned to the Argument-based Modeling(AbM) strategy, one class was assigned to the Argument-based Modeling and peer-assessment(AbM-P) strategy and one class was assigned to the Argument-based Modeling and peer- and self-assessment(AbM-PS) strategy. The results of the post modeling ability of the three groups showed that the average of the AbM-PS group with peer-assessment and self-assessment was 50.89, and the average of the AbM-P group with peer-assessment was 43.89, only the AbM group applied the discussion (F = 5.299, p

Symposium : **EDU2-4**
Chemistry Education for the Science Gifted Students
Room 605, FRI 16:05
Chair: Sukjin Kang (Jeonju National University of Education)

Boyle’s Law in History of Science and Science Education

Mi Young Han

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

Many experiments are introduced to explore the concept of Boyle’s Law. However, comparatively there is few to be interested in the formation process of that law. How did Boyle discover the law? The story started in Italy. A few Italian natural philosopher studied why the water 10m under the surface could not be pumped up. The drawings at that time showed the scene how they installed the 10m high glass tube filled with water beside the building. The length of the glass tube was reduced from 10m to 1m by Torricelli and this manageable instrument made it possible to spread the experiment to other region in Europe. The space made in the top of Torricelli’s tube was the center of the interest. “Is it filled with something or not?“ The Torricelli’s experiment was the only way to produce the mysterious space, so they should have made the instrument to explore the mysterious space. Through these experiments, the two contradictory models for air pressure, pressure by mass and pressure by elasticity, were contended. These two concepts still coexist to explain air pressure. In England Henry collected data changing the ratio of mercury and air in glass tube. However, he could not analyzed the data only by measuring the height of mercury. J tube that were designed Boyle made it possible to measure the air pressure and volume independently and it was resulted in Boyle’s Law. The air pump that produce the mysterious space initiated the debate between political philosopher Hobbes and natural philosopher Boyle for making knowledge.In this story, people, instruments, philosophy were appeared, and these showed the Boyle’s law is the result of activities of people. This story can enhance the contextual understanding of scientific knowledge emphasized in natural science curriculum.

Symposium : **ENVR-1**
Current Trends in Environmental Energy
Room 602, THU 15:40
Chair: Wooyul Kim (Sookmyung Women's University)

Highly effective nanoporous materials for hydrogen isotope separation

Hyunchul Oh

Department of Energy Engineering, Gyeongnam National University of Science and Techn, Korea

Deuterium is widely used for numerous applications such as nuclear fusion, non-radioactive isotopic tracing, neutron scattering as well as a host of others. Extracting deuterium from hydrogen isotopes mixture is, however, difficult business since its isotopes share similar size and shape. Conventional separation method such as thermal diffusion and centrifugation tends to be time and energy intensive. The development of a cost-effective separation method is therefore required.In this study, quantum sieving effect for isotope separation of light gas using Metal-organic frameworks (MOFs) is discussed. The mechanism of isotope separation by quantum effects is quite different from the normal separation by size exclusion. The isotope separation is possible when quantum effects become significant; which can be observed if the difference between entrance pore diameter and size of the molecule become comparable to the De Broglie wavelength. When decreasing the pore diameter close to molecule size, the zero-point energy can overcompensate the attraction of the wall, leading to an energy barrier for molecules entering the pore. This barrier is greatest for the molecule with the highest zero-point energy. Owing to this effect, at low temperature heavier isotope molecules are diffusing faster than lighter molecules, resulting in kinetic isotope quantum molecular sieving. Additionally, D2/H2 selectivity is only inferred from the isotherm of pure hydrogen and pure deuterium which would be different from D2/H2 mixture due to its surface adsorption competition. Therefore, recent experimental results of the kinetic isotope quantum molecular sieving effect in equilibrium and kinetic adsorption of H2/D2 mixture on MOFs will be presented in here.

Symposium : **ENVR-2**

Current Trends in Environmental Energy

Room 602, THU 16:10

Chair: Wooyul Kim (Sookmyung Women's University)

Impact of atmospheric deposition on the East Sea and the Northwestern Pacific Ocean.

Tae-Wook Kim

Environmental Science and Ecological Engineering, Korea University, Korea

Atmospheric deposition of nitrogen is an important external nitrogen source for the ocean. Amospheric concentrations and depositional fluxes of inorganic nitrogen, and factors affecting them were investigated in an eastern coastal site (Uljin) of South Korea. Potential sources for inorgnic nitrogen species could be identified based on air mass backward trajectories and stable isotope ratio in atmospheric nitrate. Atmospheric nitrogen deposition could contribute to approximately two percents of phytoplankton production in the southwestern East Sea. The nitrogen and oxygen isotopic ratios in atmospheric and seawater samples also could show a significant contribution of atmospheric nitrogen deposition to the nitrogen pool in the East Sea. In addition, airborne particles were collected in the Northwestern Pacific Ocean, and its contribution to phytoplankton productivity was similar to that found in Uljin site.

Symposium : **ENVR-3**
Current Trends in Environmental Energy
Room 602, THU 16:40
Chair: Wooyul Kim (Sookmyung Women's University)

How marine phytoplankton help cool the Earth: Dimethyl Sulfide

Ki-Tae Park

Division of Polar Climate Sciences, Korea Polar Research Institute, Korea

Ocean biology may influence the Earth’s climate through its effects on atmospheric composition due to the release of various organic compounds into the atmosphere. Dimethyl sulfide (DMS) is mostly produced by marine phytoplankton and is the most abundant form of biogenic sulfur released into marine atmosphere. Sulfur-containing aerosols provide an important source of cloud condensation nuclei in marine atmosphere. The production of sulfate from the oxidation of DMS was proposed as a negative feedback mechanism by which phytoplankton can modulate the properties of marine clouds. As Arctic and Antarctic warming occurs in the future, the decrease in sea ice may alter the abundance and species composition of phytoplankton. These changes may cumulatively have cascading effects on oceanic DMS emissions and sulfur aerosol formation. We recorded and analyzed the atmospheric DMS mixing ratios at a remote Arctic location (Svalbard; 78.5°N, 11.8°E) during phytoplankton bloom periods and found varying regional relationships between the atmospheric DMS and the extent of exposure of the air mass to the phytoplankton biomass in the ocean surrounding the observation site. Furthermore, the connection between DMS and the formation of aerosol particles in the Arctic atmosphere was evaluated by analyzing atmospheric DMS mixing ratio, aerosol particle size distribution, aerosol chemical composition and S-isotope ratio data. The results showed that the formation of submicron sulfate aerosols was significantly associated with an increase in the atmospheric DMS mixing ratio. It also confirmed that the increase in DMS-derived sulfate occurred concurrently with the formation and growth of aerosol particles.

Symposium : **ENVR-4**

Current Trends in Environmental Energy

Room 602, THU 17:10

Chair: Wooyul Kim (Sookmyung Women's University)

Intrinsic chemical transformation of iodine species in ice and its implications

Kitae Kim

Korea Polar Research Institute, Korea

Ice is ubiquitous around us and one of the dominant reaction media in nature. In general, the rate of chemical reactions decreases when temperature drops according to Arrhenius Equation($k=A\cdot e-EA/RT$). However, it was reported that the chemical reactions in ice can be markedly accelerated compared to those in aqueous solution. Iodine compounds in atmosphere play important roles on atmospheric oxidative capacity, ozone depletion event in troposphere, new particle formation, and consequently link to climate change. It was observed that the high concentration of halogen compounds including iodine in austral spring in Antarctica but the exact mechanism and sources are not clear. It was known that the biological activity can produce the atmospheric iodine species but this cannot fully explain the high amount of iodine species in Antarctic atmosphere. Therefore, we investigated the chemical of abiotic production mechanism of iodine species in ice phase. Here, I will introduce experimental results for the enhanced redox transformation of inorganic iodine species(I^-, IO_3^-) into reactive iodine forms(I_2, I_3^-) such as 1)enhanced oxidation of iodide(I^-) in ice to produce molecular iodine(I_2) and tri-iodide(I_3^-), 2)nitrite-induced activation of iodate(IO_3^-) into I_2 in frozen solution. The detailed experimental conditions and mechanism will be discussed in the presentation.

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

Oral Presentation for Young Polymer Scientists

Room 606, THU 09:45

Chair: Changsik Song (Sungkyunkwan University)

Study of Burn-In Loss in Green Solvent-Processed Ternary Blended Organic Photovoltaics derived from UV-Crosslinkable Semiconducting Polymers and Nonfullerene Acceptors

Junwoo Lee, Hae Un Kim[1], Hyuntae Choi[1], Daehwan Lee[1], Sungjin Park[2], Taiho Park*

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

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

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

This work deals with the investigation of burn-in loss in ternary blended organic photovoltaics (OPVs) prepared from a UV-crosslinkable semiconducting polymer (P2FBTT-Br) and a non-fullerene acceptor (IEICO-4F) via a green solvent process. The synthesized P2FBTT-Br can be crosslinked by UV irradiation for 150 s and dissolved in 2-methylanisole due to its asymmetric structure. In OPV performance and burn-in loss tests performed at 75 °C or AM 1.5G sun illumination for 90 h, UV-crosslinked devices with PC71BM show 9.2% of power conversion efficiency (PCE) and better stability against burn-in loss than pristine devices. The frozen morphology resulting from the crosslinking prevents lateral crystallization and aggregation related to morphological degradation. When IEICO-4F is introduced in place of a fullerene-based acceptor, the burn-in loss due to thermal aging and light soaking is dramatically suppressed because of the frozen morphology and high miscibility of the nonfullerene acceptor (18.7% -> 90.8% after 90 h at 75°C and 37.9% -> 77.5% after 90 h at AM 1.5G). The resulting crosslinked device shows 9.4% of PCE (9.8% in chlorobenzene), which is the highest value reported to date for crosslinked active materials, in the first green processing approach.

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

Oral Presentation for Young Polymer Scientists

Room 606, THU 10:00

Chair: Changsik Song (Sungkyunkwan University)

Anionic Polymerization of Azidoalkyl Glycidyl Ethers and Its Post-Polymerization Modification

Joonhee Lee, Byeong-Su Kim[1,*]

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

Polyethers like poly(ethylene glycol) have been widely used for a variety of valuable applications, though their functionalization still poses challenges due to the absence of functional handles along the polymer backbone. Herein, a novel azide-functionalized glycidyl ether monomers are presented as a universal approach to synthesize functional polyethers by post-polymerization modification. The azidoalkyl glycidyl ethers (AEGE, ABGE and AHGE) were synthesized by a two-step substitution reaction. Organic superbase-catalyzed anionic ring-opening polymerization can proceed under mild conditions compatible with an azide-pendant group, affording well-controlled azide-functionalized polyethers through high monomer conversion. The azide pendant groups on the resulting polymers were readily modified to a variety of functional groups via copper-catalyzed azide-alkyne cycloaddition reactions and Staudinger reduction. Furthermore, copolymerization of AHGE with allyl glycidyl ether was demonstrated to provide an additional orthogonal functional handle. We anticipate that this work provides a new platform for the preparation of diverse functional polyethers.

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

Oral Presentation for Young Polymer Scientists

Room 606, THU 10:15

Chair: Changsik Song (Sungkyunkwan University)

Tuning the Pore Characteristics of Hyper-Cross-Linked Polymer by Selective Removal of Alkylsilyl Groups

Jeonghyeon Lee, Myungeun Seo[1,*]

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

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

Hyper-cross-linked polymers (HCPs) are widely used microporous polymers due to their high specific surface area and small pore size (< 2 nm). HCP is readily synthesized by employing Friedel-Crafts alkylation of aromatic compounds. Poly(vinylbenzyl chloride-co-divinylbenzene) P(VBzCl-co-DVB) has been a well-known precursor enabling control of pore characteristics by varying the precursor compositions and hyper-cross-linking conditions. However, the primitive extent of control offered by previous methodologies does not meet increasing demands for straightforward and fine control of micropore size and porosity. We propose that microporoous space can be templated by a bulky pendent group such as trimethylsilyl, and its removal can create size-controlled microporous void. Here we discuss synthesis of HCPs from precursors containing different alkylsilyl groups and evaluate structure-property relationship between the alkylsilyl group and the pore characteristics toward finely tunable HCPs.

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

Oral Presentation for Young Polymer Scientists

Room 606, THU 10:30

Chair: Changsik Song (Sungkyunkwan University)

Predicting colorant usages in engineering plastic using machine learning methods

Jungup Park

Chemicals R&D Center, Samyang Corporation, Korea

Engineering plastic has been integral to modern human way of life and used prevalently from electronics to automotive applications. Among many advantages in utilizing engineering plastic, one of the key benefits is its colorability. Polymer resins can be offered in various colors via using different plastic colorants prior to processing such as extrusion. Processing conditions such as extruder temperature profile do affect the final color; but most importantly, the type and amount of colorants have the most dominant influence. Expressing the desired color in the specified engineering plastic plays a huge role in accelerated and efficient plastic processing. In order to expedite the coloring process, we propose a data-driven method which predicts the type and amount of colorants used. First, we explored the numerical relationship between the visible reflectance spectra from the specimen and the compound recipe composed of base resins, plastic additives and colorants. Second, we developed a machine learning method that predicts the plastic colorant usage given the compound recipe. The predictions from the data-driven model were assessed by comparing with the experimental results.

Oral Presentation : **INOR.O-1**
Oral Presentation of Young Inorganic Chemistry
Room 302, THU 09:00
Chair: Minyoung Yoon (Kyungpook National University)

New Precursors for Transparent Conducting Oxide Thin Film Transistor by CVD/ALD

Seong Ho Han, Bo Keun Park[1], Seung Uk Son, Taek-Mo Chung[2,*]

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Transparent conducting oxide (TCO) is an important material having high transmittance and low resistivity in the visible light region. It is widely used in applications such as photovoltaics, gas sensors, thin film transistor (TFT) and flat panel display. Mainly, group d10 metal oxides (e.g., In2O3, Ga2O3, ZnO, CdO, and SnO2) are good candidates for TCO materials because of their high mobility, which originates from the overlap of the atomic orbitals comprising the conduction band. Several methods are used to deposit TCO thin films. Among them, chemical vapor deposition (CVD) and atomic layer deposition (ALD) can accurately control the film thickness and chemical composition, and target film properties can be easily achieved. However, the ALD and CVD processes require reactive precursors for successful film deposition. This necessitates the design and development of new precursors as the first step to ensure successful deposition.In this presentation, we demonstrate synthesis of new tin and zinc precursors for depositing TCO TFT. In order to develop new precursors, the strategy with different ligands on each metal was used to control the reactivity in the deposition process. The newly synthesized compounds were analyzed by nuclear magnetic resonance, Fourier transform infrared spectroscopy (FT-IR), elemental analysis (EA), thermogravimetric analysis (TGA), mass spectroscopy and single crystal X - ray diffraction analysis.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 09:10

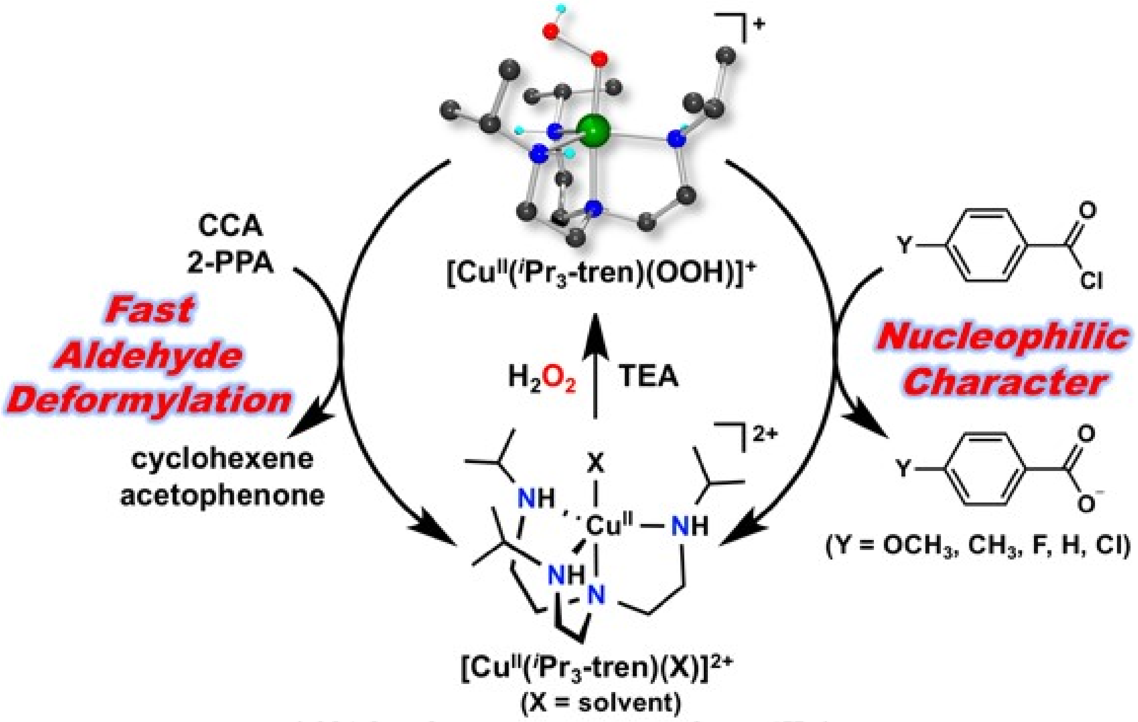
Chair: Minyoung Yoon (Kyungpook National University)

First observation of nucleophilic reactivity for a copper(II)-hydroperoxo complex

Bohee Kim, Jaeheung Cho[1,*]

Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Emerging Materials Science, DGIST, Korea*

Copper(II)-hydroperoxo species are often detected as key intermediates in metalloenzymes and biomimetic compounds containing copper. However, the only reactivity has previously been observed for the copper(II)-hydroperoxo complexes is electrophilic, occurring through the O-O bond cleavage. Herein, we report that a mononuclear end-on copper(II)-hydroperoxo complex, which has been successfully characterized by various physicochemical methods including UV-vis, rRaman, CSI-MS and EPR, is a very reactive oxidant that utilizes a nucleophilic mechanism. In addition, DFT calculations fully support the electronic structure of this complex as a copper(II)-hydroperoxo complex with trigonal bipyramidal coordination geometry. A positive Hammett ρ value (2.0(3)) is observed in the reaction of copper(II)-hydroperoxo complex with para-substituted acyl chlorides, which clearly indicates nucleophilic character for the copper(II)-hydroperoxo complex. The copper(II)-hydroperoxo complex is an especially reactive oxidant in aldehyde deformylation with 2-PPA and CCA relative to the other metal-bound reactive oxygen species reported so far. The observation of nucleophilic reactivity for a copper(II)-hydroperoxo species significantly expands the known chemistry of metal-reactive oxygen species.


]+
CCA
2-PPA
Fast Aldehyde Deformylation
cyclohexene
acetophenone
[Cu^II(^iPr3-tren)(OOH)]+
H2O2
TEA
Y
O
Cl
Nucleophilic Character
O
O−
(Y = OCH3, CH3, F, H, Cl)
]2+
X
NH
Cu^II
NH
NH
N
[Cu^II(^iPr3-tren)(X)]2+
(X = solvent)

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 09:20

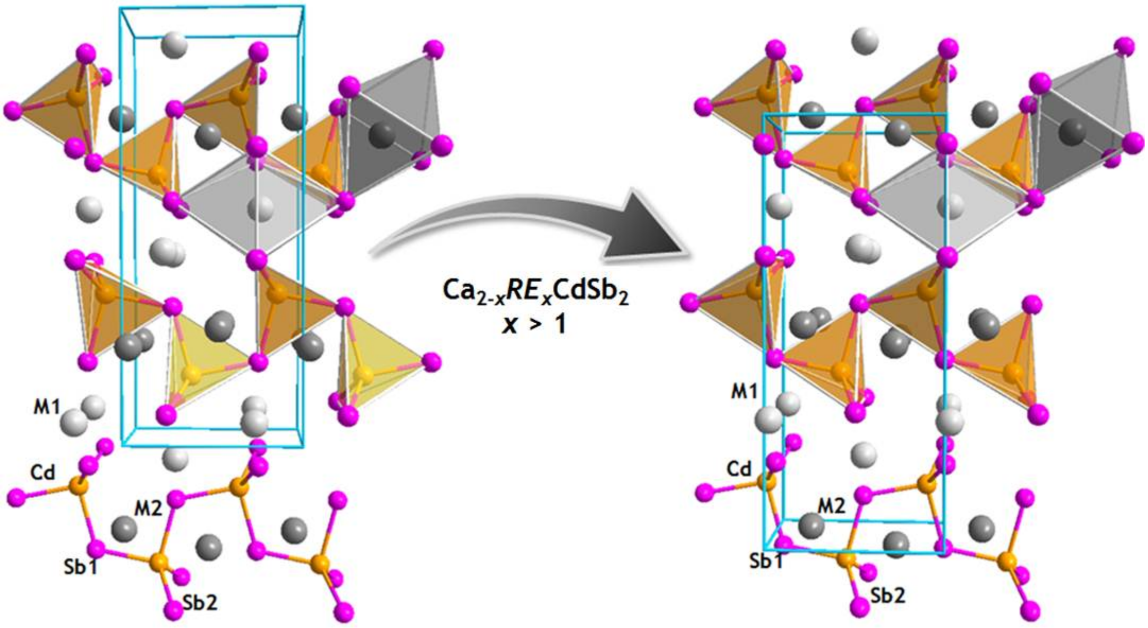
Chair: Minyoung Yoon (Kyungpook National University)

Chemical Driving Force for Phase-Transition in the $Ca_{2-x}RE_xCdSb_2$ (RE = Yb, Eu; $0.11(1) \leq x \leq 1.36(2)$) System

Ki Won Kim, **Tae-Soo You**[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Total of nine solid-solution Zintl phases in the $Ca_{2-x}RE_xCdSb_2$ (RE = Yb, Eu; $0.11(1) \leq x \leq 1.36(2)$) system with two types of cationic mixtures have been synthesized by the Pb metal-flux method, and their crystal structures have been characterized by powder and single-crystal X-ray diffraction (PXRD and SXRD) measurements. In particular, a series of solid-solution $Ca_{2-x}Yb_xCdSb_2$ ($0.43(2) \leq x \leq 1.36(2)$) compounds showed a phase-transition from the Ca_2CdSb_2-type to the Yb_2CdSb_2-type structure, both of which were very similar but slightly different homotypic structure types, depending upon the Ca^{2+}/Yb^{2+} mixed-ratio. On the other hand, the three compounds in the $Ca_{2-x}Eu_xCdSb_2$ ($0.11(1) \leq x \leq 1.04(2)$) system crystallized only in the Yb_2CdSb_2-type phase regardless of the Eu amounts. The observed phase-transition in the $Ca_{2-x}Yb_xCdSb_2$ system can be attributed to the two kinds of stacking sequence of the octahedral $[(Ca/Yb)Sb_6]$ building block and the resultant interatomic interactions between two neighboring Ca^{2+}/Yb^{2+} mixed-sites in two distinctive structure types. Moreover, according to SXRD refinements, two types of mixed-cations of Ca^{2+}/Yb^{2+} or Ca^{2+}/Eu^{2+} showed noticeable site-preferences between two available atomic sites. To understand the driving force for this phase-transition and the origin of the cationic site-preference, a series of DFT calculations using the TB-LMTO-ASA method was conducted, and the resultant DOS, COHP, and ELF diagrams were thoroughly interrogated. In particular, the COHP analysis successfully revealed that the observed phase-transition was triggered by the energetically unfavorable shorter (Ca/Yb)1-(Ca/Yb)1 interaction in the Yb-rich Ca_2CdSb_2-type phase. Moreover, the cationic site-preference in the $Ca_{2-x}Yb_xMCdSb_2$ system can be explained by the electronic-factor criterion based on the Q value of each site, whereas that in the $Ca_{2-x}Eu_xCdSb_2$ system should be elucidated by the size-factor criterion based on the size of cationic elements. The chemical compositions and the appearance of selected single-crystals were analyzed by EDS and SEM, and the thermal stability of a sample was also checked by TGA analysis.



(a) Ca_2CdSb_2-type

(b) Yb_2CdSb_2-type

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 09:30

Chair: Minyoung Yoon (Kyungpook National University)

Photodriven Water Oxidation by *p*-Benzoquinone Derivatives with an Iron Catalyst as a functional model of Photosystem II

Young Hyun Hong, Yong-Min Lee[1], Wonwoo Nam[*], Shunichi Fukuzumi[2,*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Osaka University, Japan*

Photoirradiation of a solution containing *p*-benzoquinone derivatives (X-Q) as plastoquinone analogs, a nonheme iron(II) complex, $[(N4Py)Fe^{II}]^{2+}$ (N4Py = *N*,*N*-bis(2-pyridylmethyl)-*N*-bis(2-pyridyl)methylamine), and H_2O afforded the O_2 evolution and the formation of the corresponding hydroquinone derivatives (X-QH_2) quantitatively. During the photodriven water oxidation by X-Q, $[(N4Py)Fe^{II}]^{2+}$ was oxidized by the excited state of X-Q (^{3}X-Q*) to produce the iron(IV)-oxo complex, $[(N4Py)Fe^{IV}(O)]^{2+}$, quantitatively. The concentration of $[(N4Py)Fe^{IV}(O)]^{2+}$ remained virtually the same during the repeated cycles of photodriven water oxidation by X-Q. $[(N4Py)Fe^{IV}(O)]^{2+}$ was further oxidized by ^{3}X-Q* to $[(N4Py)Fe^{V}(O)]^{3+}$, which is proposed as an active oxidant that affects the water oxidation. The photocatalytic mechanism of the water oxidation by X-Q with $[(N4Py)Fe^{II}]^{2+}$ was clarified by detecting intermediates using various spectroscopic techniques, such as transient absorption and electron paramagnetic resonance measurements. The present study reports the first example of a functional model of Photosystem II (PSII) using X-Q as plastoquinone analogs in the photocatalytic water oxidation.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 09:40

Chair: Minyoung Yoon (Kyungpook National University)

Ammonia Adsorption in a Hydrogen-Bonded Organic Framework with S-shaped Isotherm

Dong Won Kang, Minjung Kang, Hyojin Kim, Jong Hyeak Choe, Daewon Kim, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Although ammonia is a very useful chemical ingredient for fertilizer and pharmaceutical product, recent researches have suggested it as one of sources of secondary fine dust in rural areas and the amount of gas should be reduced to protect human's health. To effectively diminish the gas, several porous materials have been investigated, but most porous materials have low working capacity with type I isotherm due to high adsorption enthalpy. In contrast, an adsorbent with S-shaped gas isotherm can exhibit high working capacity in pressure-swing adsorption process. On the best of our knowledge, the adsorbent has been not explored. Herein, we synthesize and analyze a new hydrogen-bonded organic framework that can adsorb NH_3 uniquely in an S-shape fashion. The framework can be easily regenerated at room temperature with recyclability in pressure-swing adsorption protocol. Detailed experimental data and explanations will be given in the presentation.

Oral Presentation : **INOR.O-6**
Oral Presentation of Young Inorganic Chemistry
Room 302, THU 09:50
Chair: Hyunseob Lim (GIST)

S-doping in IrO_x as a Stability Enhancement Factor for Oxygen Evolution Reaction

Jun Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Clean and efficient hydrogen production is expected to be in demand in the near future to secure environment-friendly resources of energy. Among various methods, water electrolysis is considered viable with appropriate catalysts to drive the two key reactions, namely, hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In particular, due to the sluggish kinetics of OER, developing highly efficient and durable electrocatalysts for OER is essential and iridium oxide has been the benchmark owing to its intrinsically excellent catalytic activity. Despite its low natural abundance and high cost, researches for Ir-based electrocatalysts have been consistently reported to improve the efficiency of Ir. However, the deterioration of OER performance for a prolonged operation under harsh OER condition has remained as a formidable challenge until recently. Therefore, it is utterly necessary to develop strategies to secure the desired catalysts stability under electrochemical operation. We have found that in situ S doping in IrO_x leads to the enhanced catalyst stability toward OER under acidic media, and I will discuss in detail the unusual S-doping induced stabilization of the IrO_x.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 10:00

Chair: Hyunseob Lim (GIST)

Synthesis of Quinolinol-Based Indium Luminophores and Their Optical Properties

Sang Woo Kwak, Yongseog Chung, Kang Mun Lee[1], Myung Hwan Park[2,*]

Department of Chemistry, Chungbuk Natioanl University, Korea

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

[2]*Department of Chemical Education, Chungbuk Natioanl University, Korea*

Since the first example of tris(8-hydroxyquinolinato)aluminum (Alq3) by Tang and Van Slyke in 1987 as a green emitter, continuous efforts have been made to search for useful organometallic luminophores based on quinolinate derivatives to widen their applicability in various optoelectronic fields. To date, studies on systematic substitution at the C2- or C5-position in the quinolinate ligand to manipulate the HOMO–LUMO energy levels have mainly been investigated. Although such a strategy has been extensively examined, a detailed investigation of the optical properties induced in the variation of the number of quinolinate units has not been reported. We thought that the sequential introduction of multi-quinolinate units into the metal center could give rise to synergistic effects on photophysical properties and provide significant insight into the relationship between the number of ligands and the luminescent properties of the corresponding quinolinol-based organometallic luminophores.Herein, we investigated a series of indium quinolinates using a combination of experimental and theoretical techniques. In this oral presentation, the detailed synthetic aspects and photophysical properties of all the compounds (Inq1, Inq3, and InMeq1–InMeq3) will be presented.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 10:10

Chair: Hyunseob Lim (GIST)

Dimeric Aluminum Catalysts for the Synthesis of Cyclic Carbonates at Room Temperature and Atmospheric CO2 Pressure

Yoseph Kim, Youngjo Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Several catalysts for converting CO2 into cyclic carbonates at room temperature and 1 bar CO2, have been reported. In particular, aluminum, the most abundant metal in the earth's crust (the metals are in the order Al, Fe, Ca, Na, K, Mg, and Ti), is a very attractive metal for this study due to its low cost, low toxicity and high Lewis acidity. However, only a few examples of efficient non–toxic catalysts with aluminum metal centers capable of operating at ambient temperature and 1 bar CO2 are known. Typically, non–toxic Al–based catalysts require catalyst loading (> 2.5 mol%) and a long reaction time (24 h) to reach a high conversion to styrene carbonate under ambient conditions. Their catalytic activities are in the range of TON = 8.4–39.2 and TOF = 0.63–3.73 h–1. Thus, the development of new, more active Al–based catalytic systems that allow lower catalyst loading (< 1.0 mol%) and a high TON (> 100) under ambient conditions is needed. The detailed synthesis, characterization, and catalytic activities at ambient conditions of new dimeric aluminum catalysts will be discussed.ReferenceYoseph Kim, Kyunglim Hyun, Duseong Ahn, Ran Kim, Myung Hwan Park,* and Youngjo Kim* "Efficient aluminum catalysts for the chemical conversion of CO2 into cyclic carbonates at room temperature and atmospheric CO2 pressure" ChemSusChem 2019, 12, doi: 10.1002/cssc.201901661.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 10:20

Chair: Hyunseob Lim (GIST)

Data-Driven Discovery of New Zeolitic Imidazolate Frameworks

Soochan Lee, Seungyun Han[1], Seulchan Lee[1], Yongchul Chung[2,*], Wonyoung Choe[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Pusan National University, Korea*
[2]*Division of Chemical and Biomolecular Engineering, Pusan National University, Korea*

The discovery of new advanced materials is important for sustainable future. Traditionally, the materials discovery rely heavily on synthetic scientists through repeated trial-and-error experiments. Theorists commonly utilized the large-sized materials database to seek the optimal materials for desired properties. Such computational approach has been quite successful in revealing the performance limits of porous materials, but often extremely difficult to predict which materials could be synthesizable from the millions of candidates. We hypothesize that collective structural signatures, extracted from known porous solids, could be served as structural descriptors, which then could be efficient data filters for screening porous materials. In this presentation, we show not-yet-synthesized ZIF topologies, filtered and modelled from both real and hypothetical zeolite databases. To filer the entries in these databases, we have identified three structural descriptors. Together with these new candidate topologies for ZIFs, we also suggest possible synthetic strategies to realize these future ZIFs.

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

Oral Presentation of Young Inorganic Chemistry

Room 302, THU 10:30

Chair: Hyunseob Lim (GIST)

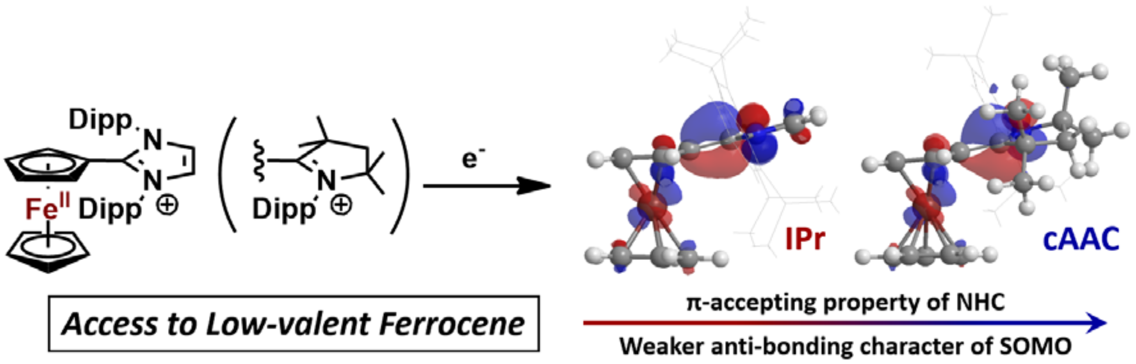
Low valent ferrocenes: stabilization by *N*-heterocyclic carbene-modified cyclopentadienyl ligands

Hayoung Song, Eunsung Lee[1,*]

Center for Self-Assembly and Complexity (CSC), Institute for Basic Science (IBS), Korea

[1]Department of Chemistry, Pohang University of Science and Technology, Korea

N-heterocyclic carbene-functionalized ferrocenes (NHC-Fcs) are obtained by oxidative nucleophilic substitution of ferrocenium with NHCs. The NHC-Fcs show a metal-to-ligand charge-transfer (MLCT) transition from iron to empty p-orbital of NHCs. The electrochemical properties of NHC-Fcs confirm the quasi-reversible NHC-Fc/$[\text{NHC-Fc}]^{\bullet -}$ cycle indicating the feasibility of low valent ferrocene species. Here, we report the first low valent ferrocene stabilized by NHC-functionalized cyclopentadienyl ligands (NHC-Cps), which is not accessible with simple ferrocene. Theoretical studies on these low valent ferrocenes clearly demonstrate the origin of their thermodynamic stability based on the orbital interaction between iron and NHC-Cp. Interestingly, the NHC-Fc can be applied for the redox-flow battery as an analyte. These low valent ferrocene species will deepen our understanding of electrochemical behaviors of ferrocenes and open the way to a rational design of low valent ferrocene derivatives.



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

Oral Presentation for Young Physical Chemists

Room 600B, THU 09:00

Chair: Young-Sang Youn (Yeungnam University)

Hydrogen-Bonding-Mediated Enhancement in Nitrogen Electroreduction Reactions on Biomimetic $Cu_{2-x}S$ Catalysts

Min-Cheol Kim, Sang Soo Han*

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

In this presentation, we introduce novel $Cu_{2-x}S$ catalysts that show greatly enhanced electrochemical activity for nitrogen reduction reaction (NRR) via hydrogen-bonding between the catalysts and the reaction intermediates, and following a biomimetic NRR pathway. The unusual electrochemical activity of various $Cu_{2-x}S$ electrocatalysts is thoroughly validated with a variety of experimental procedures. We investigate the origin of this unintuitive enhancement in NRR activity using density functional theory (DFT) simulations. Using the computational hydrogen electrode method, we compare the NRR pathway of the most promising $Cu_{2-x}S$ catalyst with the reaction pathway on Cu (111) and Fe (110) slabs. The results reveal that the N-H-S hydrogen bonding immensely stabilizes the NRR intermediates on the $Cu_{2-x}S$ surface, which leads to a large drop on limiting potential for NRR compared to Cu (111) slabs. In addition, the N-H-S hydrogen bonding enables multiple pathways for NRR on the Cu2-xS surface, resulting in increase of effective active-sites for the NRR, which hasn’t been observed in pure-metal catalysts like Fe. Finally, we show that the NRR pathway on $Cu_{2-x}S$ catalyst mimics the NRR pathway on the nitrogenase enzyme, which results in very low limiting potential compared to pure metal catalysts.

Oral Presentation : **PHYS.O-2**
Oral Presentation for Young Physical Chemists
Room 600B, THU 09:15
Chair: Young-Sang Youn (Yeungnam University)

Photooxidation Mechanism of Atomically Thin Magnetic Semiconductor $CrPS_4$

Suhyeon Kim, Sunmin Ryu[*]

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

Many two-dimensional (2D) semiconductors represented by transition metal dichalcogenides have tunable optical bandgaps in the visible or near IR-range standing as a promising candidate for optoelectronic devices. Despite this potential, however, their photoreactions are not well understood or controversial in the mechanistic details. In this work,[1] we report a unique thickness-dependent photoreaction sensitivity and a switchover between two competing reaction mechanisms in atomically thin chromium thiophosphate ($CrPS_4$), a 2D antiferromagnetic semiconductor. $CrPS_4$ showed a threshold power density two orders of magnitude smaller than that for MoS_2 obeying a photothermal reaction route. In addition, reaction cross section quantified with Raman spectroscopy revealed distinctive power dependences in the low and high power regimes. Based on optical in-situ thermometric measurements and control experiments against O_2, water, and photon energy, we proposed a photochemical oxidation mechanism involving singlet O_2 in the low power regime with a photothermal route for the other. We also demonstrated a highly effective encapsulation with Al_2O_3 as a protection against the destructive photoinduced and ambient oxidations. Reference[1] S. Kim, J. Lee, G. Jin, M.-H. Jo, C. Lee and S. Ryu, “Crossover between Photochemical and Photothermal Oxidations of Atomically Thin Magnetic Semiconductor $CrPS_4$”, Nano Lett. 2019, 19, 4043-4051.

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

Oral Presentation for Young Physical Chemists

Room 600B, THU 09:30

Chair: Young-Sang Youn (Yeungnam University)

Surface study of removal mechanism of fine dust causatives by using photocatalyst-coating on commercial products

Soong Yeon Kim, Byeong Jun Cha, Saqlain Shahid, Shufang Zhao, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Recently, the emission of VOCs (volatile organic compound), NOx, and SOx from automobile, power plant, boiler etc. was increased as a result of industrialization progress. The gases are causative materials of fine dust which has emerged as important environmental issue. Among the studies aimed to reduce fine dust concentration of atmosphere, the use of photocatalysts has been drawing much attention over the past decade. But the application of photocatalysts to various materials and actual environment is still challenging for the removal of the causative materials of fine dust. Therefore, this study shows real application of paint mixed with photocatalysts in actual environment and the mechanism of removal of the causative materials was identified by surface analysis methods.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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

Oral Presentation for Young Physical Chemists

Room 600B, THU 09:45

Chair: Young-Sang Youn (Yeungnam University)

The Thermodynamic Behavior of Surfactant into Ceramides and Phospholipids Membranes: A Molecular Dynamics Simulation Approach

Yeonho Song, Hyonseok Hwang*

Department of Chemistry, Kangwon National University, Korea

Surfactants are widely used in the daily necessities such as cosmetic products, shampoo, toothpastes, detergents etc. To offer insight into the structural and dynamic behaviors of surfactant molecules used in cosmetics at the atomistic level, we investigated the dynamics of sodium laureth sulfate (SLES) surfactants in ceramide and in 1,2-dimyristoyl-*sn*-glycero-3-phosphorylcholine (DMPC) bilayers systems using molecular dynamics (MD) simulations. We also performed the potential of mean force (PMF) calculations of the SLES monomer inserting into the ceramide and DMPC bilayers. The SLES micelle simulations reveal that several SLES molecules transfer from the micelle to ceramide bilayers while those events are not observed in the case of DMPC bilayers. The MD simulations also show that a SLES monomer easily inserts into ceramide bilayers while the molecule fails to enter into the DMPC bilayers. The PMF profiles demonstrate that a SLES monomer has a deeper free energy well of -7.1 kcal/mol in the ceramide bilayers as compared with -4.6 kcal/mol in the DMPC bilayers.

Oral Presentation : **PHYS.O-5**
Oral Presentation for Young Physical Chemists
Room 600B, THU 10:00
Chair: Young-Sang Youn (Yeungnam University)

Packaging process of DNA determines its ejection rate

Chung Bin Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

DNA ejection and packaging processes are related to each other in terms of DNA conformation inside the viral capsid. As the DNA becomes jammed, it cannot undergo dramatic conformational change in the capsid. That is, final conformation after packaging should be correlated with the conformation right before ejected. Then, a scientific question remains; whether a packaging process affects its ejection rate or not. In this work, we find three regimes which show different trends of ejection rate depending on its packaging rate; (1) knot dominant regime, (2) non-equilibrium dominant regime and (3) effective-ejection regime (intermediate regime). We carry out Langevin dynamics simulations of a semi-flexible single chain made of 660 monomers. We packages 640 monomers of a chain with different packaging rates and perform ejection simulations subsequently. If packaging rate of DNA is slow enough to be knotted itself, its ejection process becomes slow (~35%) due to knots. In this regime (1), the faster the packaging occurs, the faster the DNA is ejected due to lower knot probability. However, if DNA is packaged too fast to relax its conformation, its ejection rate decreases (~20%). In this regime (2), ejection rate gets slower as the packaging rate gets faster. Then, if a packaging rate is moderate (3), where DNA can relax enough but cannot be knotted with complex knots, DNA ejects faster than regime (1) and (2). In this regime, the ejection rate is not changed significantly depending on its packaging rate. As a result, DNA ejection rate show a non-monotonic function depending on the packaging rate. These results show that ejection dynamics is determined by its history of packaging and suggest that there could be most effective packaging rate for ejection process in nature.

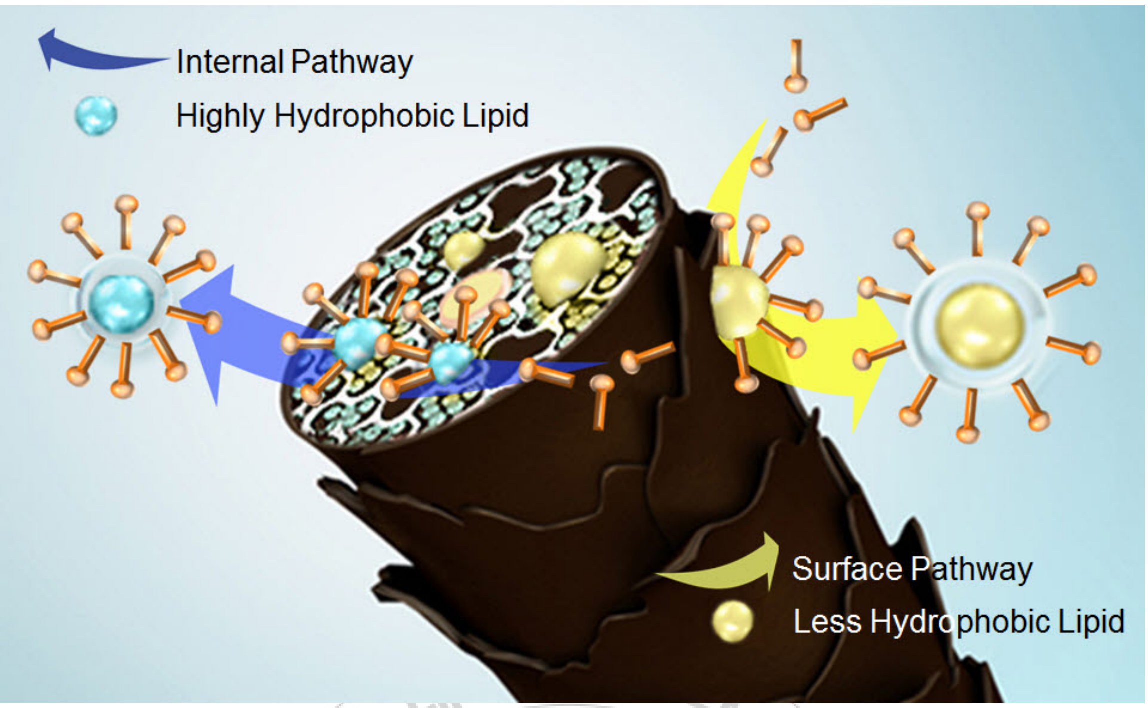
Oral Presentation : **PHYS.O-6**
Oral Presentation for Young Physical Chemists
Room 600B, THU 10:15
Chair: Young-Sang Youn (Yeungnam University)

Dual Mechanism of Lipid Loss from Human Hair

Sang-Hun Song

LG Household & Health Care Ltd., Korea

This study aims to understand the mechanism of lipid loss from hair upon contact with surfactants. We herein propose that the process of lipid loss can be categorized into two mechanisms.1) In the first mechanism, the lipids inside hair diffuse through the cell membrane complex (CMC) to the outermost layer of hair and are removed by a roll-up mechanism. In the second mechanism, the surfactant that penetrates hair directly emulsifies the lipids. The mechanism of lipid loss depends on the relative hydrophobicity of the lipid. Highly hydrophobic lipids, such as squalene and wax esters, are primarily lost through the penetration pathway, while relatively less hydrophobic lipids, such as fatty acids and cholesterol, follow the roll-up mechanism. These mechanisms were validated by confirming that surface and internal modifications of hair protected different types of lipids from the surfactant treatment. This study will be the basis for understanding the mechanisms by which surfactants damage the lipid barrier of tissues and for establishing strategies to defend the barrier.1) S.-H. Song, et. al. "Prevention of lipid loss from hair by surface and internal modification" Sci. Rep. 9, (2019) 9834


Internal Pathway
Highly Hydrophobic Lipid
Surface Pathway
Less Hydrophobic Lipid

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

Oral Presentation for Young Physical Chemists

Room 600B, THU 10:30

Chair: Young-Sang Youn (Yeungnam University)

Visible light-responsive Fe-loaded TiO_2 photocatalysts for total oxidation of acetaldehyde

Saqlain Shahid, Byeong Jun Cha, Soong Yeon Kim, Shufang Zhao, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Photocatalysis over TiO_2 is one of the most popular approaches due to the cost effectiveness and chemical stability of TiO_2. Since photocatalytically active anatase TiO_2 has a wide band gap (~3.2 eV), it is efficient under UV light irradiation but not under visible light. Various amount of Fe were loaded on as-received TiO_2 by using temperature controlled vapour deposition and the resulting structures were subsequently annealed at 750 ^{o}C. As-received TiO_2 which was almost photo-catalytically inactive for decomposition of acetaldehyde under visible light showed huge activity after loading small amount of Fe. High performing Fe loaded TiO_2 photocatalysts can be prepared by fine control Fe content since higher loading of Fe forms larger iron oxide particles which support non-radiative recombination of the excited electron-hole pairs eventually reducing the photocatalytic activity. Moreover reaction mechanism comprising of fast oxidation of acetaldehyde into CO_2 and a slower path via acetic acid to CO_2 where almost no evolution of secondary pollutant took place is also discussed.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:00

Chair: Tae-Young Kim (GIST)

Peroxidase-mimetic catalytic activity of dendrimer-encapsulated Pt nanoparticles for bioanalyses

Youngwon Ju, Joohoon Kim*

Department of Chemistry, Kyung Hee University, Korea

In this presentation, we present the peroxidase-mimetic activity of dendrimer-encapsulated Pt nanoparticles (Pt DENs) for H_2O_2-mediated oxidation of chromogenic substrates and enhanced chemiluminescence (CL) of luminol/H_2O_2. Specifically, we found that Pt DENs exhibit peroxidase-like activity catalyzing the H_2O_2-mediated oxidation of 3,3’5,5’-tetramethylbenzidine (TMB) to blue-colored products. We also synthesized Pt DENs having different sizes with sub-nanometer accuracy by adjusting the stoichiometry between the dendrimer and complexed precursor Pt ions. The Pt DENs exhibited size-dependent catalytic activity for the highly enhanced CL of the luminol/H_2O_2 due to the peroxidase-like activity of Pt DENs. The size-dependent catalytic activity of Pt DENs was ascribed to the different chemical states of the Pt DENs as well as to their different surface areas depending on their sizes. A brief description of how the peroxidase-mimetic catalytic activities of Pt DENs could be utilized for various analytical applications is also provided.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:03

Chair: Tae-Young Kim (GIST)

Digital rectilinear ion trap mass spectrometer

Jae-ung Lee, Han Bin Oh*

Department of Chemistry, Sogang University, Korea

We present the demonstration of digital rectilinear ion trap (RIT) mass spectrometer. We designed and manufactured the RIT based on the design of Ouyang et al. For the operation of this mass analyzer, we applied concepts of the digital ion trap, in which RF voltages of the rectangular waveform was applied to the electrode, not typical sign waveform. Besides, the mass scan is also done by frequency scan, not by voltage scan. In this research, we used the FPGA controller for the generation and control of the rectangular waveform. Circuits composed of two high power/RF MOSFETs were also made to generate trapping voltages. All I/O communication was controlled by home-built LabVIEW software. We plan to conduct the performance experiment of this mass spectrometry in detail and expand it for more sophisticated analyses.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:06

Chair: Tae-Young Kim (GIST)

Near-Infrared Molecularly Imprinted Polymers-Based Sensor for Ultrasensitive Detection of Pharmaceutical Residues in wastewater

Mohamed Ragab Elsayed Ali, Salah Mahmoud Tawfik Ahmed, Yong-Ill Lee*

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One of the alternative techniques for determining pharmaceuticals and their metabolites in the aquatic environment is the use of molecularly imprinted polymers (MIPs) as recognition systems. MIPs are tailor-made artificial receptor sites in a polymer, which possess good affinity and selectivity. This work presents the design of new optical sensor-based MIP for the detection of Carbamazepine (CBZ) as one of the most frequently detected pharmaceutical residues in wastewater. MIP was prepared via *in situ* photopolymerization process using upconversion nanoparticles (UCNPs), CBZ, N-allyl-3,4,5-trihydroxybenzamide, (E)-N-acryloyl-3-(3,4-dihydroxyphenyl)acrylamide and 1-(carboxymethyl)-4-vinylpyridin-1-ium bromide, ethylene-glycol dimethacrylate, eosin Y/ triethylamine (TEA) as fluorescent materials, template, functional monomers, cross-linking agent, and an initiating system, respectively. Our method utilizes the internal visible light emitted from UCNPs upon photoexcitation with near-infrared radiation, to locally photopolymerize a thin polymer shell of the MIP around the UCNPs. The TEM images of this hybrid showed an ultrathin shell of 2.5 nm thickness. Under optimum conditions, the results of the fluorescence quenching analysis showed excellent sensitivity (LOD, 28.5 pM) with good linear ranges of 0.5 nM to 500 μM for CBZ and a correlation coefficient of 0.992. Moreover, the practical application of the developed sensor for CBZ detection in tap and river water samples has been successfully described with satisfactory recoveries of 98.24-104.23% and RSD less than 5%. This work offers a novel facile strategy to develop a fluorescent sensor with selective, rapid and accurate detection of CBZ in the wastewater.

Keywords: molecular imprinting polymer, *in situ* photopolymerization, UCNPs, CBZ.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:09

Chair: Tae-Young Kim (GIST)

A study on the concentration change of inorganic arsenic in rice by the various pretreatment

DongChan Lee, Sang-Ho Nam[1,*]

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IARC under the WHO classifies arsenic as a carcinogen in Group I. We are exposed to arsenic mainly from the drinking water and food, and the chronic exposure can cause the problems such as peripheral nerve disease. Thus, the accurate determination of total arsenic and arsenic species in rice has been an important issue. In particular, the major arsenic species in rice was found to be the inorganic arsenic which was highly more toxic than the organic arsenic.If we can reduce the inorganic arsenic in rice by using the great pretreatment before cooking, it can help people to reduce the risk. Thus, this study was focused on the pretreatment methods that could reduce the content of inorganic arsenics in rice. The pretreatment methods were washing, soaking (for 24 hours), ultrasonication (for 90 minutes).Inorganic species in rice was separated by ion chromatography, then determined by inductively coupled plasma mass spectrometry. Arsenobetaine was used as an internal standard. The concentration of inorganic arsenic in rice that was without the pretreatment process was 94.2 μg/kg (± 10.7 μg/kg). The concentration was decreased to 43.6 (41.8 μg ± 3.77 μg/kg), 62.7 (66.2 μg/kg ± 2.8 μg/kg), 80.7 % (77.5 μg/kg ± 8.38 μg/kg) by the soaking of rice in water for 24 hours, the ultrasonication of rice for 90 minutes, and the washing of rice in water, respectively.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:12

Chair: Tae-Young Kim (GIST)

Voltammetric layer-by-layer biosensor for metabolite in human serum

Yunpei Si, Hye Jin Lee*

Department of Chemistry, Kyungpook National University, Korea

The metabolite level in human body is associated with the health condition and disease status. An electrochemical layer-by-layer (LbL) biosensing platform was demonstrated for highly sensitive and selective determination of metabolite by self-assembly of oppositely charged layers on screen printed carbon electrode (SPCE) surface. The developed sensing platform was applied in both normal human and myocardial infarction patient serum samples. The sensing results were further validated by a commercial detection kit and liquid chromatography-mass spectrometry (LC-MS) technique.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:15

Chair: Tae-Young Kim (GIST)

Synthesis, dispersion, tribological performance of alkyl functionalized graphene oxide as an oil lubricant additive and synergistic effect with WS$_2$

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

Department of Chemistry, Keimyung University, Korea

Graphene and WS$_2$ has been reported as an excellent lubricant additive for reducing adhesion and friction, when coated on the various surfaces as an atomically thin material with low surface energy. GO is various methods have been proposed to enhance the physical properties of GO by its reduction, because it is difficult to apply GO to hydrophobic lubricant due to the large numbers of oxygen functional groups and the remarkably poor physical properties. To solve this problem First, We have painted a long alkyl chain of graphene oxide (GO) to improve the dispersion of oil-based lubricants with greatly enhanced lipophilicity. Second, a gelator is used for dispersion to improve lubrication performance. Alkyl functionalized GO is synthesized by reacting NH2-GO with butyl chloride, hexyl chloride, octyl chloride, decyl chloride, dodecyl chloride, tetradecyl chloride in ethanol under reflux, then 0.1wt% of alkyl functionalized GO are added into the base oil (PAO oil) and oil which containing WS$_2$. and then, ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene is investigated by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), and Scanning electron microscope (SEM). The tribological tests are performed with a tribometer via ball-on-disk test mode.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:18

Chair: Tae-Young Kim (GIST)

Digital and Absolute Quantification of Microdroplets using Wide-Field Imaging System for real-time Droplet Sorting

Sunghyun Ki, Dong-Ku Kang[1,*]

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Droplet-based microfluidics (DMF) have been developed as a digital assay that allow precise and absolute quantification of targets such as enzyme, bacteria and nucleic acid. To avoid complex and expensive optic system as a detector, CCD sensors and smartphones have been integrated with DMF to image droplets. Here, we introduce digital CFU assay for absolute quantification of living-bacteria using 50.6-megapixel CMOS sensor which allow imaging the area of 10 cm2. Detectable number of droplets depends on the diameter of droplets, and it can be calculated as 9.29×106, 5.8×105 or 1.5×105 droplets when droplets are generated as 10, 40 or 80 μm in diameter, respectively. In this approach, 107 droplets can be analyzed within one minute after being generated and digital CFU assay was performed as a proof of concept study for the absolute quantification of living bacteria without fluorescent labeling. As a wide-field imaging system, 100 mm macro and full-frame 50.6-megapixel CMOS sensor-integrated digital camera were used to image droplets, and droplet images were analyzed using Matlab that simultaneously analyzes five individual colors. Bacterial cells (E.coli) were encapsulated within droplets as a single cell manner using microfluidic device and phenol-red was co-encapsulated as a pH indicator to detect living bacteria. In addition, we have investigated the migration of ammonia gas from bacteria and colorimetric dye between droplets. Interestingly, the dye was not able to across between the droplets but ammonia gas permeated through the droplets. Here, we introduce a detection platform (wide-field imaging system) that can be used for the monitoring large number of droplets (up to 107) within 5 minutes.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:21

Chair: Tae-Young Kim (GIST)

Separation of exosomes and lipoproteins in human serum using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Exosomes play an important role in maintaining homeostasis and intercellular communication in body fluids and are known to be associated with physiological and pathological functions. Recently, exosomes are expected as a biomarker for disease prognosis and diagnosis. In particular, a number of studies have shown that blood exosomes are closely related to cancer. Lipoproteins carry lipids through the blood stream and are classified according to its size and density. Because of the similarity in their size and density of lipoproteins, it is important to separate exosomes and lipoproteins from bloodField-flow fractionation (FFF) is an analytical technique that is capable of separating nano to micron sized particles in an aqueous solution in an empty channel space without packing materials. In this study, exosomes and lipoproteins in human serum were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) using field programming and monitored by a series of UV and multi-angle light scattering (MALS) detectors. During separation, fractions of exosome and lipoprotein were collected and analyzed by Western blot, transmission electron microscope (TEM), and nUPLC-ESI-MS/MS for proteomic.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:24

Chair: Tae-Young Kim (GIST)

Reducing Process of Silica Particle by Metallothermic Reduction Reaction

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Recently, metallothermic reduction reactions (MRRs) are displacement reactions that use reactive metals to reduce nonmetal materials, mainly silicon and carbon, particularly in their nanostructured forms obtained using an MRR with magnesium as the reductant. Here, we mixed magnesium/aluminum with anisotropic Au@SiO2 core-shell nanoparticles and heated it up to 650℃ to reducing silica shell. We found that small parts scattered in the silica shell were found to be converted to silicon with crystallinity in early time in the heating process. And the reaction progresses, it became porous silicon shell with anisotropic gold nanoparticles as a core structure. It shows that reduction reaction starts inside the silica particle such as island and it proceeds to around. Finding the optimal conditions, this core-shell nanoparticle could be used for dual imaging in bio-healthcare applications.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:27

Chair: Tae-Young Kim (GIST)

Chemiluminescent probes-based paper strips for detection of influenza

Jinsol Han, Sharipov Mirkomil, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

According to the World Health organization (WHO), millions of people are infected by influenza virus each year. Traditional diagnosis methods require high cost equipment and technician for diagnosis of influenza virus. Last decade, the development of alternative diagnosis techniques for influenza has received a tremendous attention of scientist. The emerging paper-based analytical devices (μPAD) has shown their potential as low cost and easy to use method in detection of several toxic molecules. Moreover, the availability as renewable natural resources of natural cellulose fibers, low cost, recyclability, and the possibility to modify the surface of the paper with sensing molecules such as fluorescent probe or chemiluminescent is promising in development of novel, low-cost and easy to operate sensing material. Unlike fluorescent probes, the emerging chemiluminescent probe do not require light excitation, resulting in higher sensitivities and signal-to-noise ratios. In this work, we aim to develop chemiluminescent derivative-based μPAD that is selectively activated in the presence of influenza virus. μPAD was designed via stacked system to ensure to deliver the influenza virus to the target area after deposition onto μPAD.**Keywords:** chemiluminescent,μPAD,infulenza,detection

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:30

Chair: Tae-Young Kim (GIST)

Application of SERS active AuNPs-MOF nanocomposite for sensitive detection of MGITC

Anupam Das, Namhyun Choi[1], Kyoung Neon Kim, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

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

The current project is aimed to investigate the Surface-Enhanced Raman Scattering (SERS) properties of a nanocomposite (AuNPs-MOF) of gold nanoparticles (AuNPs) and Metal (Fe) Organic Framework (MOF), MIL-101(Fe)-NH2. Upon finding the SERS activity of the AuNPs-MOF nano composite, we found its applications in detecting trace amount of target protein transferrin (Tf) in spiked phosphate buffer saline (LOD: 1 nmol) and human serum (LOD: 0.625 μmol) samples. It was observed that upon increasing Tf concentration, overall SERS intensity of AuNPs-MOF-Tf complex gets enhanced significantly. Eventually, we established a calibration curve (SERS intensity vs Concentration of Tf) to find out the Total (or Transferrin) Iron Binding capacity (TIBC) values of unknown samples. Considering the normal TIBC level (~1.7 to ~3.7 g/L) of a healthy human being, we can calculate the TIBC value of given samples. TIBC values indicate whether the patients are suffering from iron deficiency.KEYWORDS: Surface-Enhanced Raman Scattering (SERS); SERS-active nanocomposite, Transferrin

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:33

Chair: Tae-Young Kim (GIST)

Plasmonic Sensing of Pyridine by Chemical Interface Damping of Single Au/Ag Core Shell Nanorods.

Kyeong Rim Ryu, Ji Won Ha[1,*]

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

Noble metal nanoparticles have a unique optical property resulted from localized surface plasmon resonance (LSPR). In this study, we observed that the thicker the silver coated in Au/Ag core shell nanorods, the broadener the line width of LSPR under dark-field scattering microscopy and spectroscopy. The chemical interface damping (CID) is one of the plasmon decay processes in gold nanoparticles. Herein, to find new plasmonic metal that can induced CID as an alternative to gold nanorods, we conducted an dark -field (DF) scattering studids of Au/Ag core shell nanorods with pyridine as adsorbate. We investigated the CID induced by a pyridine attached on the Au/Ag core shell hybrid nanorods under dark-field scattering microscopy and spectroscopy. By the adsorption of pyridine molecules on the Au/Ag nanorods, their LSPR linewidth was broadened with decreasing the scattering intensity due to CID effect.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:36

Chair: Tae-Young Kim (GIST)

Probing Structural Change of Protein using Small-angle X-ray Scattering (SAXS) and Cross-linking Mass Spectrometry

Chae Eun Heo, Chae Ri Park, MyungKook Son, Sooyeon Chae, Min Ji Kim, Paul Valery Migisha Ntwali, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Probing the protein-protein interactions are crucial for the study of wide variety biological system. Numerous research has been reported that various methods are developed to support the identification, characterization and analysis of protein complexes. Since the protein-protein interactions are influenced by PTM, metal ions, ion concentration has been reported that charged species abundant in our body (e.g. metal ion, DNA, nucleic acid, heparin, glycosaminoglycans etc.) influence to the mechanism of amyloid fibrillation by electrostatic interaction. Here, we have studied to understand the molecular mechanism of protein fibrillation under ATP, which is a small biological polyanion and is present in high levels in cell. Firstly, we have conducted the thioflavin T(ThT) assay which monitors the formation of amyloid fibril. To identify and characterize the protein complexes between protein and small molecules, we have utilized electrospray ionization mass spectrometry (ESI-MS) and ion mobility spectrometry (IMS), along with circular dichroism (CD) and solution small-angle x-ray scattering (SAXS). The experimental evidence obtained from these diverse analytical techniques, and subsequent studies about biological anion-mediated protein aggregation would be highly helpful in understanding the mechanistic details of amyloid fibrillation under the influence of external factors, which affect protein-protein interactions.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:39

Chair: Tae-Young Kim (GIST)

Synthesis and Biodegradation Evaluation of Biodegradable Microcapsules for Medical and Industrial Applications

Jiwon Kim, Donghyeok Jo[1], Youngbok Lee[2,*]

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

Microcapsules are materials used in various fields such as medicine, cosmetics, and fabric softeners, and microcapsules are often synthesized into microplastics in household goods. However, as plastics are the main culprit of ecosystem destruction and environmental pollution, many countries are declaring war on plastics around the world. Therefore, we attempt to synthesize biodegradable microcapsules and check their biodegradation in various ways. We selected biodegradable polymers through theoretical investigations and synthesized cellulose-based microcapsules using biodegradation studies of NMR-based cellulose using enzymes. Synthesis of microcapsules was confirmed by microscopy, IR and NMR, and residual isocyanates that may remain during microcapsule synthesis were analyzed by IR and NMR to check for harmlessness to the human body. To confirm the biodegradability of the synthesized microcapsules, we performed BOD, COD and cellulase-based degradation experiments.The enzymic study was measured by NMR, UV spectrum, and SEM, and the change over time was confirmed. The biodegradation of microcapsules could be predicted through the change of line width, absorbance, and morphology. The biodegradability tendency of the samples shown by each experiment did not deviate significantly from the expectations based on the raw material used for the synthesis. Currently, we are conducting more various control experiments, focusing on experiments to verify whether the changes caused by cellulase are correct, and trying to develop biodegradation confirmation methods applicable to microcapsules that will be useful in medicine and industry.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:42

Chair: Tae-Young Kim (GIST)

lipidomic analysis of serum from mice exposed to ambient particulate matter using LC-MS approach

Seoyoung Jang, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Ambient particulate matter(PM) has known as environmental risk factors in Korea, and associated with disease including asthma, cardiovascular and nervous disorder. However, the molecular mechanism by exposure to PM has not been fully understood.. We observe the metabolic perturbations in response to PM with a diameter 2.5-10 µm (PM10) exposure in mouse model. In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3 weeks in chambers. We conducted untargeted lipidomic analysis of serum from mice to evaluate metabolic perturbations using ultra performance liquid chromatography/quadrupole time of flight mass spectrometry (UPLC/Q TOF MS). Partial least squares - discriminant analysis (PLS-DA) score plots showed a clear separation between the PM10 exposed group and control group. We observed changes in lipids including ceramide, free fatty acid, acylcarnitine, phospholipid and diacylglycerol species in PM10 exposed mice compared to control. phospholipid species were decreased in PM10 exposed group compared to control, whereasacylcarnitine and free fatty acid species were significantly increased in PM10 exposed group, indicating the alteration in fatty acid oxidation metabolism. This study demonstrates that the LC-MS based-lipid profiling can be a used to understand the metabolism of PM10 exposed group on biological system.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:45

Chair: Tae-Young Kim (GIST)

Multiple omics analysis related to mesenchymal stem cell mass cultivation

Seung-Eun Lee, Min-Sik Kim[1,*]

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

Biotechnology products and medicines based on stem cells are being developed in variety. The development of stem cell bioproducts and therapies require a large amount of stem cells. In order to develop such products, it is necessary to process a culture system capable of mass production of stem cells. We carried out experiments with the aim of developing technology to monitor stem cell culture markers through quantitative analysis of metabolites and proteins related to cell growth and proliferation. “Additive A” was inserted into the control media to develop a medium in which the proliferation rate of stem cells was fast and the morphology of the cells were not altered. The mesenchymal stem cells were cultured for 5 time points (6 hours, 1 day, 2 days, 3 days, and 4 days) in the new media which is added Additive A and the control media. As a result, it was found that glutamine and sugar were consumed more in the new media than in the control media, and this shows that the cells of the new media required more energy which is needed for cell proliferation. Proteome quantification was performed by clustering the ratio of the control media to the new media according to the time points. As a result, we observed biological processes and KEGG pathways related to Additive A in the cluster which show a decreasing pattern over time. We conclude that Additive A is involved or helps in cell proliferation.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:48

Chair: Tae-Young Kim (GIST)

Lipidomic analysis of elaiosomes from Coreanomecon hylomeconoides Nakai by high performance liquid chromatography- tandem mass spectrometry

Hyejin Park, Tae-Young Kim[*]

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

Elaiosome is a small structure attached to a seed and mainly consists of lipids. The main role of elaiosome is to attract ants to disperse the seeds of plants from place to place. High performance liquid chromatography-electrospray ionization-tandem mass spectrometry (HPLC-ESI-MS/MS) was used to profile and quantify the lipid contents in the elaiosomes of Coreanomecon hylomeconides Nakai, which is endemic species in Korea. Lipids extracted from elaiosomes sampled in seven different populations were subjected to relative quantification using a quadrupole-time-of-flight mass spectrometer in both positive and negative ion modes. More than 85 lipid species including glycerophospholipids and triglycerides were identified in each of pooled samples analyzed in triplicate. The majority of fatty acyl chain composition of the identified lipids were C16:0, C16:1, C18:1, and C18:2, These results were consistent with the previous studies on the composition of elaiosome free fatty acids, which are regarded as key players in the mutualistic relationship between and ants. Finally, statistical analyses were conducted with the R software to differentiate lipidome among the seven populations.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:51

Chair: Tae-Young Kim (GIST)

Novel $ZnBi_2O_4$-graphite Composites as Highly Active Visible-Light Photocatalyst for the Mineralization of Rhodamine B

Truong Thi Thuy, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Novel photocatalyst from composite of zinc bismuth oxide ($ZnBi_2O_4$) and graphite hybrid composites was prepared via a co-precipitation method. The photodegradation activity of prepared $ZnBi_2O_4$-graphite hybrid composites were tested on rhodamine B (RhB) solutions under visible-light irradiation. The prepared composite exhibited excellent photocatalytic activity, leading to more than 95% of RhB degradation at an initial concentration of 50 mg.L^{-1} with 1.0 g catalyst per liter in 150 min. The excellent visible-light photocatalytic mineralization of $ZnBi_2O_4$-1.0graphite in comparison with pristine $ZnBi_2O_4$ may be attributed to synergetic effects, charge transfer between $ZnBi_2O_4$ and graphite, and the separation efficiency of the photogenerated electrons and holes. The results demonstrate the feasibility of $ZnBi_2O_4$-1.0graphite as a potential heterogeneous photocatalyst for environmental remediation.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:54

Chair: Tae-Young Kim (GIST)

Size fractionation of Graphene Oxide by Asymmetrical Flow Field-Flow Fractionation

Myoungjae Ko, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Graphene is known to have surprising properties including electrical, thermal and mechanical properties. However, graphene still has many problems with applications on the market, because of low solution dispersibility and poor processability. To solve these problems, graphene oxide liquid crystal (GOLC) was discovered. In contrast to graphene, GOLC is a two-dimensional graphene-based material that has a good processability at large scales and is well dispersed due to the liquid crystal characteristics, therefore, it is expected to be utilized for the various applications. However, GO has a wide size distribution due to various factors in the synthesis step. GO size distribution needs to be controlled because it relates to the liquid crystal characteristics of GO. Many studies have been conducted to solve the problem of wide size distribution of graphene oxide, but it has not been solved effectively yet. These studies pose problems with size separations that modify graphene oxide. This study was aimed to find an optimal condition for the size-based separation of GO using asymmetrical flow-field fractionation (AF4). For the confirmation of size separation, fractions GO were collected and analyzed using scanning electron microscopy (SEM) and optical microscopy (OM). As a result, GO in plate form can beseparated by hyperlayer separation mode of AF4 with the recovery of GO within 70% to 90%.

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

Oral Presentation of Young Analytical Chemists I

Room 600A, THU 09:57

Chair: Tae-Young Kim (GIST)

MS-based analysis of 2D and 3D spheroids neuroblastoma cells to explore mechanisms underlying cellular heterogeneity in neuroblastoma cell models.

Paul Valery Migisha Ntwali, Chae Eun Heo, MyungKook Son, Sooyeon Chae, Min Ji Kim, Chae Ri Park, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

MS-based proteomics of 3D cell model and single cell system has been extremely successful for quantitation of proteins that are integral components of essential processes for life and continues to revolutionize protein characterization. Development in different areas of proteomic workflow such as sample preparation, MS instrumentation and data processing have enabled us to get comprehensive information from MS-based proteomics. However, exploring cellular heterogeneity in tumors continues to be a challenge among researchers using cell models. Development of 3D cells has increased our understanding of cellular heterogeneity in tumor cells, an achievement which has caused the shift of recent researches towards the use of 3D cell culture. In this study, we optimized 3D spheroids cell culture condition by adjusting 3D scaffold and incubation conditions. Furthermore, we performed a comparative study of 2D and 3D spheroids cells by evaluating differences in anti-cancer drugs toxicity in these cell models. Additionally, ESI-MS was employed to highlight further differences between 2D and 3D neuroblastoma cells by emphasizing on differences in drug uptake mechanisms of these 2 cell models. This study will enhance our understanding of 2D and 3D spheroid cell model impacts in optimizing the efficacy of anti-cancer drugs and will contribute to the development of pre-treatment methods of 2D and 3D spheroid model for MS-based proteomics.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:00

Chair: Hyun Joo An (Chungnam National University)

Development of an automatic sample preparation system using a Lab-on-a-Disc

Hwa-yong Jang, Han Bin Oh*

Department of Chemistry, Sogang University, Korea

A disc for the lab-on-a-disc analysis was designed and constructed to automatically perform sample preparation for quantitative analysis of formaldehyde using LC-MS/MS. This disc was designed to perform a series of well-organized sample preparation steps, such as mixing and filtering, automatically on the lab-on-a-disc. In addition, an instrument that can perform the lab-on-a-disc analysis was also made in-house, which utilized the feedback loop of several serial communications between an arduino microcontroller and a LattePanda microcomputer board to control the fluid movement and precisely measure a number of real-time revolutions. Further, a high-speed image capturing system was also implemented to monitor fluid movements.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:03

Chair: Hyun Joo An (Chungnam National University)

Luminescence from Au(0)@Au(I)-thiolate core-shell nanoclusters separated by polyacrylamide gel electrophoresis (PAGE)

Yunjeong Kang, Joohoon Kim*

Department of Chemistry, Kyung Hee University, Korea

In this study, we report photoluminescence (PL) and eletrochemiluminescence (ECL) of glutathione-stabilized Au nanoclusters (AuNCs) which are finely separated by polyacrylamide gel electrophoresis (PAGE). In our previous study, we found that the as-synthesized AuNCs having Au(0)@Au(I)-thiolate core-shell structure exhibited strong orange color PL due to the aggregation induced emission (AIE) of Au(I)-thiolate oligomers which were located in the shell of AuNCs. Interestingly, the as-synthesized AuNCs displayed near-infrared (NIR) ECL in spite of their PL primarily within the visible wavelength region (i.e., orange color PL). Herein, we pursue the further PAGE study of the as-synthesized AuNCs. The PAGE-separated AuNCs displayed different ECL and PL properties primarily due to their different chemical oxidation states. This study provides a better understanding of luminescence of the AuNCs with Au(0)@Au(I) - thiolate core-shell structure.

Oral Presentation : **ANAL2.O-3**
Oral Presentation of Young Analytical Chemists II
Room 600A, FRI 09:06
Chair: Hyun Joo An (Chungnam National University)

Application of Sensitive MRM-MS based Platform to Monitor the Non-human Sialic Acid (Neu5Gc) in Human Tissue

Nari Seo, Hyun Joo An*

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

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

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:09

Chair: Hyun Joo An (Chungnam National University)

Optical sensing of triclosan with Fluorescence of upconversion nanoparticles composed potassium permanganate

Seong-Soo Lee, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Triclosan (TCS) have been widely used in a lot of manufacturers as a preservative and a chronically toxic compound that adversely affects biological organisms and human health. In this work, optical features of upconversion nanoparticles (UCNPs) were used to develop a simple and rapid method for detecting TCS. A novel optical sensor of TCS is designed based on carboxylic group functionalized $NaYF_4:Yb^{3+}/Er^{3+}$ UCNPs coated with potassium permanganate ($KMnO_4$). The TCS sensor is able to do the non-autofluorescence, sensitive, and selective sensing through the "turn off-on fluorescence" technique by fluorescence resonance energy transfer (FRET). The FRET between the $KMnO_4$ and UCNPs occurs under an Near-infrared excitation at 980 nm resulted "turn-off fluorescence". The sensor becomes "turn-on fluorescence" with the presence of TCS because TCS reduces $KMnO_4$. Recovering the fluorescence of UCNPs has ability to detect TCS. The resulting sensor showed an excellent response to TCS with 0.2 μM of a limit of detection in optimized conditions. **Keywords:** Triclosan, UCNPs, FRET

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:12

Chair: Hyun Joo An (Chungnam National University)

Anlalyzing and switching chiral structure with magnetoplasmonic nanoparticles.

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Nanomachines are synthetic assemblies that switch between defined molecular conformations upon stimulation by external triggers. Previously, our group arranged different types of magnetoplasmonic nanoparticles into 1-3D metastructure by controlling ligands, solvent's surface tension and external magnetic field. It is well known that assembled nanoparticles made new localized surface plasmonic modes and this can be observed as light absorbance on specific wavelength and chirality of the assembled structure can be detected by circular dichroism. Recently researchers developed the concept of dynamic plasmonics which means the studies of plasmonics on nanostructure has changeable morphology. Snapshot image and spectra of moving structure is detected. The concept suggested in this presentation shows one type of 4D self-assembly which means controlling the dynamicity of the arrays of nanoparticles. Not only taking snapshots of moving nanostructures, movement of nanostructure can be remote controlled. Between two layers of 1D structured nanoarray with an angle, rotational mode of the particles between the layers can be reversibly controlled by tuning the wavenumber in that area. This work is considerable to use in tunable plasmonic devices, which can be used as nanomachines, chemical sensors and telecom applications.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:15

Chair: Hyun Joo An (Chungnam National University)

Characteristics and Electrochemical Performance of Graphene/Silicon/Carbon nanofibers Composite films as Anode Material for Binder-Free Lithium ion Secondary Batteries

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

Department of Chemistry, Keimyung University, Korea

We report the interfacial study of a Graphene/Silicon/Carbon nanofiber Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon nanofibers (CNFs) were grown via chemical vapor deposition method with an iron-copper catalysts. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 700℃, and maintained for 30 min to synthesize CNFs. GO aqueous dispersion was added into the Silicon/CNFs solution, and the mixture was sonicated for 2h to obtain a GO/Silicon/CNFs aqueous dispersion. Electrode was fabricated by flow-directed vacuum filtration of GO/Silicon/CNFs aqueous dispersion through a filter membrane (90 mm in diameter and 0.22 μm in pore diameter) followed by air drying and peeling off from the filter. Subsequently,the composited GO/Silicon/CNFs was heated up to 550℃ at a rate of 10℃ min-1 in a quartz tube furnace with an argon flow,and maintained for 2h to form a rGO/Si/CNFs composite film. The morphologies, compositions and crystal quality of the prepared rGO/Silicon/CNFs composites were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of rGO/Silicon/CNFs composites as an anode of Lithium ion secondary batteries were investigated using two-electrode coin-type cell. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:18

Chair: Hyun Joo An (Chungnam National University)

Identification multidisciplinary function and analysis active chemical compound structure of natural biological resources that were collected from Southern-east asian countries

Yeseul Park, TaeYeong Park[1], Dong-Ku Kang[2,*]

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This study aims to derive multi-function material from biological natural resources and also to identify its chemical structure. Candidate materials were collected from southern-east asian countries and one-hundred samples were provided for the screening of functional materials. First, dried samples were homogenized and extracted with 70% ethanol and then antimicrobial activity was identified using conventional ‘paper disc assay’ against infectious pathogens including *S. pseudopneumoniae*, *S. aureus*, *E. coli*, *P. mirabilis*, and *C. albicans*. Antioxidant activity was also validated by conventional ABTS(2,2′-azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid)) assay and effect of cellular ROS concentration was characterized using 'DCF-DA'-based cell staining approach. After 1st screening of antimicrobial activity with paper disc assay, IC_{50} values of derived candidates were characterized for the quantification of antimicrobial activity using alamarBlue-based cell viability assay. Finally, one of the candidates was characterized which has both antimicrobial and antioxidant activities. The IC_{50} values of X were identified as 0.294, 2.340, 2.175 and 3.699 mg/ml against *S. pseudopneumoniae*, *S. aureus*, *P. mirabilis* and *C. albicans* respectively. Moreover, the IC_{50} value of antioxidant for X was calculated as 4.157 μg/ml. Then, active chemical compound was purified by fractionation using prep-HPLC. The activities of antimicrobial and antioxidant were confirmed with paper disc-based susceptibility test and ABTS assay respectively. Finally, their cellular action mechanism and biocompatibility were also identified.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:21

Chair: Hyun Joo An (Chungnam National University)

Effective Sample Preparation of Polyphenols in Wine using Deep Eutectic Solvent-based Dispersive Liquid-Liquid Microextraction for HPLC-UV Determination

Jongsung Noh, JinSol Lee, Seung Hoon Song, Won Hoe Koo, Hyun-Woo Cho[1], Seung Woon Myung*

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Polyphenols are phytochemicals that exist in grapes and are beneficial to human health. In this study, resveratrol, oxyresveratrol and piceatannol in wine were extracted by deep eutectic solvent based on dispersive liquid-liquid microextraction (DES-DLLME), and a method for quantification these polyphenols using high performance piquid chromatograph - UV/Vis (HPLC-UV/Vis) was established. Several parameters for sample extraction, clean-up and concentration were optimized and verified by Central Composite Design (CCD) using Design Expert 11. The optimized sample preparation parameters are as follows: type and ratio of DES as extraction solvent, methyltributylammonium chloride / decanoic acid(1:3 molar ratio); type and volume of basic solvent, $KHCO_3$ and 1.3 mL; volume of acetic, anhydride, 250 μL; time of derivatization, 5min; type of dispersive solvent, methanol; ratio of extraction and dispersive solvent, 1:5.5; and salt 1.0 g. Chromatographic separation with HPLC/UV-vis was performed using Agilent HPLC 1100 series, ACME C_{18} (4.6mm id × 150 mm length, 5 μm particle size) column and gradient elution mode using water and 70% methanol. From the established extraction and HPLC-UV conditions, the limit of detection (LOD) and limit of quantitation (LOQ) of three analytes in the spiked sample were 6.09 - 11.77 μg/L and 18.47 - 35.66 μg/L, respectively. Recovery studies were performed at low, medium and high concentration range in calibration curve, and accuracy and precision in working range were 81.33 - 108.25 % and 2.03 - 10.73 RSD %, respectively. The calibration curves for the quantitative analysis were obtained the concentration range of 18.47 - 184.7 μg/L, 35.66 - 356.6 μg/L and 27.42 - 274.2 μg/L with correlation coefficient(r^2) from 0.9909 to 0.9984, respectively. The proposed method was applied to the determination of polyphenols in wine samples.

Oral Presentation : **ANAL2.O-9**
Oral Presentation of Young Analytical Chemists II
Room 600A, FRI 09:24
Chair: Hyun Joo An (Chungnam National University)

Programmable paper-based microfluidic devices with printed patterns for analytical assays

Veasna Soum, Sooyong Park, Albertus Ivan Brilian, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Regulating the flow of fluid in microfluidic devices enables a wide range of assay protocols for analytical applications. A programmable, paper-based microfluidic device fabricated by using a method of cutting and laminating, followed by printing, is reported. By printing silver-nanoparticle (AgNP) and poly[4,5-difluoro-2,2-bis(trifluoromethyl)-1,3-dioxole-co-tetrafluoroethylene] (PTFE) patterns on the surface of a paper channel, we were able to either increase or decrease the flow of fluid in the fabricated devices. By using hydrophilic AgNP patterns, we were able to increase the speed of fluid flow in the channel by up to 15 times compared to that in a pristine channel, and by using hydrophobic PTFE patterns, we were able to delay that speed by a factor of about 3. Using the programmable, paper-based microfluidic device, we demonstrated a single-step protocol for detecting glucose and a multi-step protocol for detecting methyl paraoxon (MPO). We anticipate that our programmable, paper-microfluidic device will lead to improved fluid handling techniques, which are crucial for achieving a wide range of analytical assays.

Oral Presentation : **ANAL2.O-10**
Oral Presentation of Young Analytical Chemists II
Room 600A, FRI 09:27
Chair: Hyun Joo An (Chungnam National University)

Investigation of serum lipid signatures of pig in post-hepatectomy liver failure from expanded hepatectomy using nanoflow UHPLC-ESI-MS/MS

HaeA Kim, JongCheol Lee, Myeong Hee Moon[*]

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The liver is an important organ that is involved in numerous biochemical reactions andlipid metabolism. Because the liver is an excellent regenerative organ, liver resection is usually performed when liver cancers were developed. However, hepatectomy may cause a variety of complications. The biggest contributor to mortality from liver resection is a post-hepatectomy liver failure (PHLF) which is the inability of the liver to perform its normal synthetic and metabolic functions after liver resection. Therefore, an early and quick diagnose of PHLF is still an important issue.In this experiment, pigs were divided into three groups of six laparotomized pigs (sham), seven 70% partial hepatectomized pigs (the 70% PH group), and seven 90% partial hepatectomized pigs (the 90% PH group) to obtain sera at each time points: pre-operation (PO), 14 hours (14h), 30 hours (30h), and 48 hours after the operation. The lipids extracted from sera were analyzed using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS) and 284 lipid species were structurally confirmed by collision-induced dissociation (CID) experiments. Among them, 184 lipid species were quantified by selective reaction monitoring (SRM) mode. From the statistical analysis, eleven lipids showed significant differences (> 2-fold, $p < 0.01$) between the 70% and the 90% PH groups at 30 hours after the operation. Among the lipids, TG was decreased considerably at 90% PH. PC plasmalogen was increased at 90% PH and showed significant correlation (Pearson's $r > 0.7$, $p < 0.05$) with total bilirubin (TBIL) and prothrombin time (PT) which indicate liver function.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:30

Chair: Hyun Joo An (Chungnam National University)

Control of Desired Aspect Ratio of Gold Nanorods based on Seed-Mediated Method.

Sunghoon Yoo, Seunghyun Lee[1,*]

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Seed-mediated method is a general procedure for the synthesis of gold nanorods(Au NRs) who developed Murphy et al. and El-Sayed et al. Many of the interesting optical properties of Au NRs are determined by the position of their LSPR peak, which is largely governed by the aspect ratio of Au NRs. In this experiment, we have controlled parameters to tuned from visible to infrared by tuning their aspect ratio. As a result, we show the tunable plasmon bands depending on the volume/concentration of the chemical reagents by using hydroquinone as a reducing agent in the presence of silver nitrate and the longitudinal LSPR peak is still in the range of Vis-NIR even if the size of Au NRs is less than 20nm in length. And previously known LSPR peaks of Au NRs are less than 900nm or more than 1200nm. But we also synthesize high aspect ratio Au NRs with peaks more than 1,200nm by using co reducing agent.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:33

Chair: Hyun Joo An (Chungnam National University)

Performance evaluation of SERS-PCR sensors for future use in rapid and sensitive genetic assays

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Herein, we report a surface-enhanced Raman scattering (SERS)-based polymerase chain reaction (PCR) assay platform for the sensitive and rapid detection of a DNA marker (pagA) of Bacillus anthracis. Real-time quantitative PCR (RT-qPCR) has been recently considered a gold standard for the quantitative evaluation of a gene expression level but it still suffers from the problem of a long thermocycling time. To address this issue, we developed a conceptually new SERS-PCR platform, and evaluated its performance by sequentially measuring the Raman signals of Bacillus anthracis DNA after the completion of different thermocycling numbers. According to our experimental data, SERS-PCR has lower limit of detections (LODs) than RT-qPCR under the small cycle number of 20. In particular, it was impossible to detect a target DNA amplicon using RT-qPCR before the number of cycles reached 15 but SERS-PCR enabled DNA detection after only 5 cycles with a LOD value of 960 pM. In addition, the dynamic range for SERS-PCR (0.1–1,000 pM) is wider than that for RT-qPCR (150-1000 pM) under the same condition. We believe that this SERS-PCR technique has a strong potential to be a powerful tool for the rapid and sensitive diagnosis of infectious diseases in the near future.KEY WORDS: SERS-PCR assay, low PCR cycle, Bacillus anthracis,

Oral Presentation : **ANAL2.O-13**
Oral Presentation of Young Analytical Chemists II
Room 600A, FRI 09:36
Chair: Hyun Joo An (Chungnam National University)

NMR structural studies of tIK fragment with anti-inflammatory effective

Yuyoung Song, Hyunjun Jang, Ji-Ho Jeong, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Rheumatoid arthritis is caused by an autoimmune disorder. Various immune cells such as T cells, B cells, macrophages and dendritic cells participate in the inflammatory response of RA. Initially, inflammation starts around the synovial membrane around the joint, spreading around cartilage, ligaments, and destruction. In addition, inflammation of the blood vessels and skin may lead to systemic diseases such as vasculitis, anemia, and headache. There are many causes for the disease, but one of them is known as the imbalance of pro-inflammatory cytokines and anti-inflammatory cytokines. In addition, self-antigen recognition due to abnormal major histocompatibility complex (MHC) class II-expressing B cells produces antibodies that induce more severe RA. Recent studies have showed that truncated-IK (tIK) protein`s derivatives downregulate MHC class II on activation in inflammatory diseases. Therefore, we conducted epitope research to develop tIK as a new anti-inflammatory therapeutic agent for rheumatoid arthritis patients. In our study, we examined the phosphorylation pattern of protein cell signaling by isolating macrophages from transgenic mice transplanted with the tIK nucleotide sequence. It has been reported that tIK protein phosphorylates the 496th tyrosine of interleukin 10 receptor subunit alpha and has anti-inflammatory effect. We sought to find tIK protein’s specific regions that induce phosphorylation at the interleukin 10 receptor subunit alpha. So, we predicted the possible structure of tIK based on IL-10 through sequence homology modeling and proposed 4 anti-inflammatory peptide candidates and identified the anti-inflammatory activity through the TH17 cell differentiation test. Among them, the 18-mer peptide with anti-inflammatory activity was named tIK-YK4. Afterwards, we found 9-mer and 14-mer, based on 18-mer, and anti- inflammatory effect was also confirmed. Currently, we have successfully performed overexpression using E. coli and are optimizing the purification process. And we are trying to identify the relationship between structure of these peptides and anti-inflammatory activity through NMR studies.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:39

Chair: Hyun Joo An (Chungnam National University)

An investigation on the change of inorganic arsenic concentration in Hiziki by the pretreatment method using IC-ICP-MS

Seon Hwa Lee, Sang-Ho Nam*

Department of Chemistry, Mokpo National University, Korea

The accurate determination of a toxic element in food has been important for the assessment of food safety. Accordingly the method for the reduction of toxic element in food also has been needed. Arsenic is well known as an element with high toxicity, but its toxicity depends on the chemical forms. Inorganic arsenic is more toxic than organic arsenic, thus the quantitation of inorganic arsenic in a food is critical. In particular, HIziki has been known to contain the inorganic arsenic. In this study, the determination of inorganic arsenic in Hiziki was performed, then the change of the concentration of inorganic arsenic was investigated with the various pretreatment methods of Hiziki. The inorganic arsenic was separated by ion chromatography (IC), then detected by inductively coupled plasma mass spectrometry (ICP-MS). The different pretreament methods were the soaking, steaming, and boiling the Hiziki. The concentrations of inorganic arsenic in Hiziki were reduced to 50%, 30%, 74% of the original concentration by soaking, boiling, and steaming, repectively.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:42

Chair: Hyun Joo An (Chungnam National University)

Synthesis of fluorine doped structured $Li_2FeP_2O_7$ and its electrochemical and structural characterizations

Chaewon Moon, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Lithium-ion batteries (LIBs) as attractive power source have contributed to commercial success of electronic device. The LIBs have been predominately used in portable electronic devices, and its applications have expanded into electric vehicle (EV), energy storage system (ESS) and smart-grid technology. The motivation for using a LIBs relies on its high energy density, fast charge and discharge efficiency, stable operating at strict condition, and eco-reliability. As a cathode material, lithium metal pyrophosphates, $LiMP_2O_7$ (M = Mn, Co, Fe, V), have been subjected to intense recent research. Among them, $LiFeP_2O_7$ (LFPO) shows superior ionic diffusivity, inferior electronic conductivity and structural stability due to strong P–O bond as polyanion. Therefore, anion doping into the polyanion site can be able to improve intrinsic electrochemical properties such as band gap, and enhance lithium diffusion limitations. Consequently, fluorine anion (F^-) has been selected as a dopant in for oxygen sites. The fluorine doped LFPO has been synthesized by solid state reaction method. The structural study of the material has been investigated by X-ray diffraction and ^7Li MAS NMR. And the electrochemical performances have been characterized with designed galvanostatic cycling in various C rates and cyclic voltammetry (CV) measurement.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:45

Chair: Hyun Joo An (Chungnam National University)

The targeted metabolomics profiling of urine in diabetic kidney disease using NMR

Jin Seong Hyeon, Geum-Sook Hwang*

Korea Basic Science Institute, Korea

Diabetic kidney disease (DKD) is a leading cause of end stage renal disease (ESRD), and the number of patients diagnosed with chronic kidney disease (CKD) and ESRD due to diabetes has been steadily increasing worldwide. To investigate the biomarker for CKD originated from DKD (DM-CKD), we performed the targeted metabolomics profiling using 800 MHz nuclear magnetic resonance spectroscopy (NMR). Prospectively urine samples consecutive patients with DM-CKD stage 1 to 5 (n=208) and controls (n=26) with normal kidney function were analyzed. We found a gradual elevation of glucose, mannose, fumarate, and pyroglutamate according to DM-CKD stages compared with control groups. These four urinary metabolites were significantly correlated with urinary protein-to-creatinine ratio and estimated glomerular filtration rate. After Kaplan-Meier analysis and multivariate Cox analysis, metabolites were associated with ESRD progression. This study demonstrates that the NMR based targeted-metabolomics shed light on understanding of the DM-CKD and enable us to predict the risk of ESRD progression.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:48

Chair: Hyun Joo An (Chungnam National University)

Antioxidative Activity of Oligosaccharides on UV-induced Photoaging in human skin cells

Ara Lee, Dong-Ku Kang*

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Ultraviolet (UV) is one of the major reasons for the skin aging and its intracellular action mechanisms are well-defined as 1) mitochondrial damage due to UV-induced reactive oxygen species (ROS) and 2) collagen collapse in the subcutaneous layer due to increased expression of matrix metalloproteinase (MMP). Thus, antioxidants are commonly used as an anti-aging agents to inhibit free radicals produced by UV such as ROS. Oligosaccharides are kind of carbohydrates that have various biological activities such as improving intestinal environment and immune stimulation. Recently, antioxidant activity of oligosaccharides has been also identified from few kinds of oligosaccharides. In this study, seaweed-derived oligosaccharides were identified on anti-photoaging that was induced by ultraviolet B (UVB) irradiation in human keratinocytes (HaCaT cells). Reductive activity was validated using conventional ABTS assay with nine individual oligosaccharides and result indicated that neoagarooctaose (NA8) and neoagarodecaose (NA10) have reducing power. In HaCat cell-based antioxidant experiments, NA10 also inhibits ROS formation and ERK 1/2 phosphorylation. Finally, MMP-1 production was also interfered by NA10 treatment in HaCat cells. There experimental results suggested that NA10 has a potential for the skin anti-photoaging.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:51

Chair: Hyun Joo An (Chungnam National University)

Comparison of Solvent Effects on Cytotoxicity of Pt-based Drugs in 2D Cells and 3D Spheroid Cells

Min Ji Kim, Chae Eun Heo, Sooyeon Chae, Paul Valery Migisha Ntwali, Chae Ri Park, MyungKook Son, Da Gyeong Hyun, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Cisplatin (cis-[Pt(NH3)2Cl2]), a first-generation metal-based anticancer drug, has been widely used to treat diverse cancers including pediatric cancers. Cisplatin is commonly administered as a single drug or in combination with other drugs to raise its efficacy. Nevertheless, cancer cells could have acquired or intrinsic resistance to cisplatin. For this reason, a large number of in vitro studies have been conducted to clarify the mechanism of this phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin and other drugs due to its ability to dissolve drugs in high concentration. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl-. To understand how DMSO directly impede platinum (Pt)-mediated toxicity, we employed 3 dimensional spheroids and 2 dimensional monolayer of SK-N-SH neuroblastoma cells to understand cisplatin activity in the presence of DMSO. Then we employed an inductively coupled plasma mass spectrometry (ICP-MS) for the quantitative analysis of cisplatin. Our quantitative results show that cellular uptake and DNA-Pt adduct formation is significantly reduced for the cells treated with cisplatin dissolved in DMSO compared to those treated with cisplatin dissolved in media. Overall, our study would provide valuable insight into the reduced efficacy of cisplatin for cancer treatment in the presence of DMSO, based on the correlation with structural change of cisplatin induced by DMSO.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:54

Chair: Hyun Joo An (Chungnam National University)

Hybrid Magnetic Carbon Nanoparticles for Removal Organic Dyes

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[1]*Bio-Nano Technology, Hanyang University, Korea*
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The elimination of organic dyes from the wastewater of textile and food industry companies is a serious environmental issue. Nowadays, there are numerous materials are used for organic contaminants treatment, however, they are difficult to reuse and separate. Herein, we show the fabrication of hybrid magnetic carbon nanoparticles (MCNs) with different shapes for removal the organic dyes because of facile separation and reusability. Three different shapes are multi-shell, core-shell and cross-linker and they were synthesized by polydopamine and iron precursor. The MCNs morphology, structure and surface area were confirmed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and Brunauer-Emmett-Teller (BET). Moreover, the three systems were investigated the removal efficiency. The cross-linker shape was shown the highest efficiency for adsorption the organic contaminants because of high surface area. Furthermore, the commercial activated carbon (M200) was linked with magnetic for comparing the efficiency with the cross-linker MCNs. Hence, these MCNs can perform as an excellent adsorbent with various benefits of reusability and facile separation.

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

Oral Presentation of Young Analytical Chemists II

Room 600A, FRI 09:57

Chair: Hyun Joo An (Chungnam National University)

Quantitative lipidome analysis of serum from mouse exposed to microplastic using deuterium oxide labeling

Jin Young Park, Tae-Young Kim*

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

Microplastics are small (typically less than 5 mm) pieces of plastic fragments and have become global environmental and health concerns due to pollution of the aquatic system including oceans, rivers, and lakes as well as air and soil. Most studies on the health risks caused by microplastic exposure have been conducted on marine organisms with high concentrations of microplastics. To study the in vivo effects of low concentrations of microplastics on mammal, untargeted lipidomic analysis was performed with a mouse model based on Deuterium Oxide (D_2O) Labeling for Global Omics Relative Quantification (DOLGOReQ) technique that we have recently developed. For experimental group, ICR mice were administrated with microplastics in drinking water for 5 weeks. The plastic concentration was set to consume 386.82 ng of polyethylene (PE) and polystyrene (PS) per day. Four and five replicates of mice were exposed to PS and PE, respectively. The concentration of plastic in drinking water was changed weekly based on the mouse weight. For the control groups, four replicates of ICR mouse were fed by either normal drinking water or 5% D_2O enriched drinking water. After 5 weeks, serum samples were collected from both experimental and control groups. Lipids were extracted from mouse serum using Folch method. Lipid extracts were analyzed by high-performance liquid chromatography-mass spectrometry. Finally, relative quantification of lipidome between experimental and control groups was performed by DOLGOReQ. A total of 212, 176, and 301 lipids were identified from control, PE, and PS groups, respectively. Among them, 136 lipids were commonly identified. In the relative quantitative analyses, 2 sphingomyelins in PE exposed group and 2 glycerophosphoethanolamines in PS exposed group showed significant changes compared with control group.

Award Lecture in Division : **LIFE.O-7**
Oral Presentations by Young Life Chemists
Room 301, THU 10:30
Chair: Jung-Min Kee (UNIST)

Cell Penetration of Multimeric Cationic Amphipathic Peptides at Nanomolar Concentrations

Yan Lee

Division of Chemistry, Seoul National University, Korea

Cell penetrating peptide (CPP) is one of the effective ways to deliver difficultly penetrable molecules into cells. However, most CPPs show the penetrating activity at high micromolar concentrations, limiting their practical applications. We discovered that CPPs based on multimeric alpha-helical leucine (L) and lysine (K)-rich amphipathic peptides can effectively penetrate cells at 10 nM, a 1,000-fold lower concentration than the penetrable concentrations of previous reported cell penetrating peptides (CPPs), Tat or oligo arginine. The antiparallel conformation of the LK multimer was critical for the effective penetration of the CPPs at low nanomolar concentrations. The multimeric LK-CPPs show rapid cell penetration through macropinocytosis at low nanomolar concentrations, unlike the monomeric LK, which have slower penetrating kinetics at much higher concentrations. The heparan sulfate proteoglycan (HSPG) receptors are highly involved in the rapid internalization of multimeric LK-CPPs. As proof of concepts in biomedical applications, various biomolecules were delivered into cells with bioactivities at nanomolar concentrations. The multimeric CPP can be a useful platform for the intracellular delivery of biomacromolecular reagents that have difficulty with penetration in order to control biological reactions in cells at feasible concentrations for biomedical purposes.

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

Oral Presentations by Young Life Chemists

Room 301, THU 09:00

Chair: Jung-Min Kee (UNIST)

Key Structural Determinants of the Hyper-thermostability and Global Folding of Acyl Carrier Protein from *Thermotoga maritima*

Yeongjoon Lee, Jungwoo Park, Yangmee Kim*

Department of Biotechnology, Konkuk University, Korea

Acyl carrier proteins (ACP) are the key participants of the fatty acid synthesis (FAS) systems. They carry the growing acyl intermediates within their hydrophobic pockets and shuttle them to the proper FAS enzymes. As the hyperthermophile *Thermotoga maritima* resides at extremely hot hydrothermal vents, its acyl carrier protein (*Tm*-ACP) has to maintain proper structure and function at near-boiling temperatures. Here, aiming to understand the origin of its thermostability, we determined the solution structure of *Tm*-ACP and investigated backbone dynamics using NMR spectroscopy for the first time. Mutation studies based on structure and dynamics data confirmed that extensive ionic interactions on its surface and enhanced hydrophobic packings cooperatively stabilize the structure of *Tm*-ACP, resulting in an extremely high melting point (100.3℃). *Tm*-ACP has a large hydrophobic pocket to accommodate long acyl chains required for the thermal adaptation of the cell membrane of *T. maritima*. An ionic cluster mediated by the unconserved D59 protrudes helix III outward and fixes the pocket to the open conformation. This open conformation with slow exchange near the cavity may be important for its functional plasticity. Hydrogen/deuterium exchange, thermal and chemical denaturation experiments revealed that Ile15 and Phe54 are the key residues for the folding processes of ACPs. This study provides the insights into the strategies for thermophilic adaptations and for designing proteins with optimized stabilities.

Oral Presentation : **LIFE.O-2**
Oral Presentations by Young Life Chemists
Room 301, THU 09:15
Chair: Jung-Min Kee (UNIST)

Sequestering ATP inside Mitochondria by Nucleopeptide inducing Cancer Cell death

Huyeon Choi, Ja-Hyoung Ryu[1,*]

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Adenosine triphosphate (ATP) has important roles in cellular processes such as energy production, cellular respiration, cell signaling and metabolism. Most of cancer cells have three times higher concentration of ATP compared to normal cells. By removing ATP inside cancer cells, it can result in severe effect such as apoptosis. Herein, we developed selective cancer treatment by sequestration and self-assemblies of ATP with nucleopeptide (NP). NP has nucleobase (thymine, thy) which interacts with adenine and alternative positively charged amino acids and hydrophobic amino acids which are mitochondria targeting sequence and it can self-assemble in water. NP exhibits higher binding affinity with ATP by electrostatic interaction and hydrogen bond resulting in large complex and assemblies with ATP compared to ADP. To enhance selectivity towards cancer cells, NP-ADP having nanometer-sized micelles accumulates inside cancer cells and form large assembly with ATP which has higher binding affinity by reversible interaction. Thus, sequestration of ATP and large assemblies of NP-ATP inside mitochondria cause severe effects such as the metabolic process of ATP and stress by structures towards cancer cells.

Oral Presentation : **LIFE.O-3**
Oral Presentations by Young Life Chemists
Room 301, THU 09:30
Chair: Jung-Min Kee (UNIST)

A DNA-Encoded Combinatorial Library of Macrocyclic Peptoids Targeting Skp2

Min Hyeon Shin, Hyun-Suk Lim*

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

Skp2 is frequently overexpressed in many human cancers and considered as a proto-oncogene. It is believed that Skp2 has two critical roles in tumorigenesis. The first role of Skp2 is related with proteolytic function. As a component of the SCF^{Skp2} ubiquitin E3 ligase complex, Skp2 derives the cell cycle by mediating the proteasomal degradation of key cell cycle proteins. The second role is non-proteolytic function which suppresses p53-dependent apoptosis by outcompeting p53 for binding to histone acetyltransferase p300, thereby perturbing p300-mediated p53 acetylation and leading to tumorigenesis. As a result, inhibition of Skp2 functions is emerging as a promising and novel anti-cancer strategy.In this study, we constructed a DNA-encoded one-bead one-compound cyclic peptoid library with a vast theoretical diversity of 1.13×10^7. The library was screened against Skp2 protein using FACS-based high-throughput screening method. We discovered cyclic peptoid inhibitors that directly bind to Skp2. The binding of inhibitors was confirmed in fluorescence polarization assay, and these inhibitors decreased the level of p53 and acetylated-p53 which is related with non-proteolytic function of Skp2. Our results suggest that FACS-based high-throughput screening with DNA-encoded library can be used as useful tool to get many potential hit structure of target protein, and identified Skp2 inhibitors have great potential as a chemical probe to investigate Skp2 functions and as novel drug candidates for anticancer therapy.

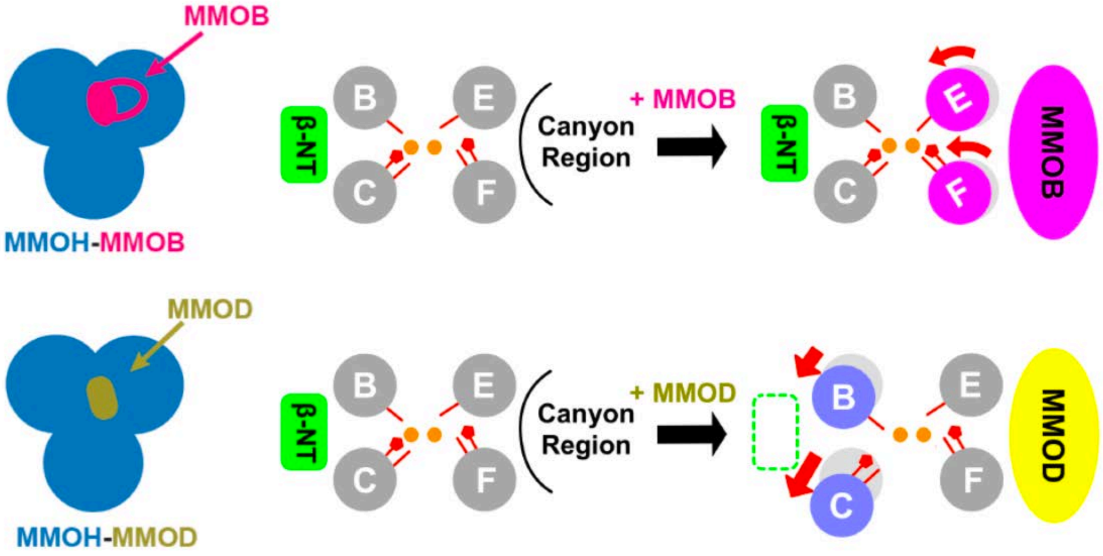
Oral Presentation : **LIFE.O-4**
Oral Presentations by Young Life Chemists
Room 301, THU 09:45
Chair: Jung-Min Kee (UNIST)

MMOD-induced structural changes of hydroxylase in soluble methane monooxygenase

Hanseong Kim, Minseok Kwak, Seung Jae Lee[1], Uhn-Soo Cho[2,*]

Department of Chemistry, Pukyong National University, Korea
[1]*Department of Chemistry, Chonbuk National University, Korea*
[2]*Department of Biological Chemistry, University of Michigan, U.S.A., United States*

Soluble methane monooxygenase in methanotrophs converts methane to methanol under ambient conditions. The maximum catalytic activity of hydroxylase (MMOH) is achieved through the interplay of its regulatory protein (MMOB) and reductase. An additional auxiliary protein, MMOD, functions as an inhibitor of MMOH; however, its inhibitory mechanism remains unknown. Herein, we report the crystal structure of the MMOH–MMOD complex from *Methylosinus sporium* strain 5 (2.6 Å). Its structure illustrates that MMOD associates with the canyon region of MMOH where MMOB binds. Although MMOD and MMOB recognize the same binding site, each binding component triggers different conformational changes toward MMOH, which then respectively lead to the inhibition and activation of MMOH. Particularly, MMOD binding perturbs the di-iron geometry by inducing two major MMOH conformational changes, i.e., MMOH β-subunit disorganization and subsequent His147 dissociate with on Fe1 coordination. Furthermore, 1,6-hexanediol, a mimic of the products of sMMO, reveals the substrate access route.


MMOB
MMOH-MMOB
β-NT
B
C
E
F
Canyon Region
+ MMOB
β-NT
B
C
E
F
MMOB
MMOD
MMOH-MMOD
β-NT
B
C
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Canyon Region
+ MMOD
B
C
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F
MMOD

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

Oral Presentations by Young Life Chemists

Room 301, THU 10:00

Chair: Jung-Min Kee (UNIST)

Mimicry of the Cytoskeleton: Actin and Microtubule Polymerization in Giant Unilamellar Vesicle causing Shape Changing

Sungwoo Jeong, ChangHo Kim[1], Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea
[1]*Institute of Biological Interfaces, Sogang University, Korea*

Microtubule and actin cytoskeletons are physically contacted in a cell and dynamically coordinated to play vital roles in many cell functions, from migration, growth, and division. These structural dynamics of cytoskeletal proteins are of interest, the physical roles of cross-linking proteins between two filaments have been identified. Yet most studies were performed in a highly controlled interface or a bulk. Recently, we developed to simulate a cytoskeleton formation through ATP-dependent actin polymerization in a giant unilamellar vesicle (GUV) Optical stimulation-initiated ATP synthesis and induced ATP-dependent actin polymerization, leading to the growth of three-dimensional highly curled actin filament network. In this study, we further added the ingredients for microtubule formation into the actin polymerizable GUV system and controlled both of the polymerization via single divalent cation Mg2+. Also, by adapting the lipid phase separation techniques in the GUV system, the GUV could bare any physical forces generated during the polymerizations. We will discuss how the lipid phase-separated GUV showed structurally and shape change during the cytoskeleton proteins polymerization. At last, we will discuss how these shape changes and the cytoskeleton co-polymerizable GUV system could lead to artificial cellular movements in future research.

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

Oral Presentations by Young Life Chemists

Room 301, THU 10:15

Chair: Jung-Min Kee (UNIST)

NIR Emissive C2V Symmetric Pyridinium Salt: Selective Discrimination Capabilities G-Quadruplexes over Canonical/Non-Canonical Nucleic Acids and Their In-Cellulo Demonstrations

Anup Pandith

Department of Chemistry, Chonbuk National University, Korea

G-quadruplexes (G4s) are non-canonical nucleic acids which can regulate various metabolic process in physiological systems. Due to its inevitable applications in genetics and therapeutics its recognitions in genome attracts great interest both chemical-biologists and genetic engineers. Considering the significance of G4s, current work we report small and highly efficient novel NIR emissive C2V symmetric pyridinium salt (1) was utilized to identify G4s in invitro as well as in in-cellulo. Rationally designed probe 1, showed selective switch-on response in NIR region (emission centred at 620 nm) without inducing any background signals from dsDNA, ssDNA, RNA and other non-canonical nucleic acids viz., triplex, three-way junction etc. Additionally, strategic design and sensing capabilities were supported through model compounds 2, 3 and 4 using UV-Vis, fluorescence, gel electrophoresis, and dynamic light scattering (DLS) studies.

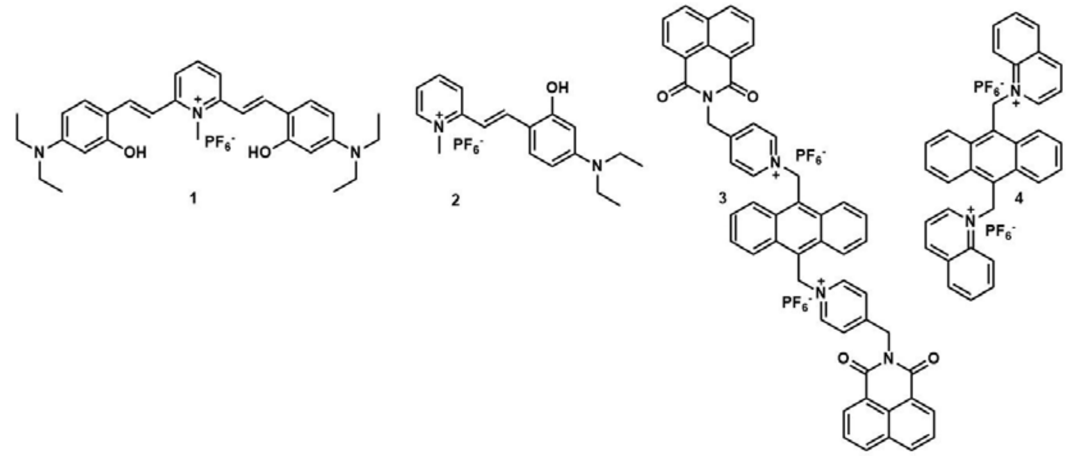


Fig. 1 Structure of fluorescent probes **1**, **2**, **3** and **4.**

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

Oral Presentations for Young Scholars in Organic Division

Room 700A, THU 09:00

Chair: Jun Hee Lee (Dongguk University)

Europium Catalysis for Aerobic Oxidation of Alcohols and Photoluminescence Tracking

Seongwoo Kim, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Lanthanide chemistry (for both catalysts and reagents) is a versatile and useful tool for traditional organic synthesis. Several important lanthanide reagents such as SmI2 and CAN (ceric ammonium nitrate) are widely used to the oxidation-reduction during organic synthesis with stoichiometric manners. For the catalytic reaction, a variety of Lewis acid catalysis has been developed using lanthanide salts such as $La(NO_3)_3$, $Sc(OTf)_3$, and etc. However, there are very limited studied for the catalytic applications of lanthanide with redox changes of metal in the literatures.[1] Europium (^{63}Eu) could have relatively stable two oxidation states (Eu(II) and Eu(III)) due to the half-filled $4f^7$ electronic configuration. We have utilized the redox cycle between Eu(II) to Eu(III) to organic transformation, especially the aerobic oxidation of alcohols to corresponding aldehydes. The redox cycle of europium was activated by the external oxidants (TEMPO, O_2, and NO_3^-) in the acidic condition, and their cycle was working for alcohol oxidation to corresponding aldehyde and not for carboxylic acid (i.e., no over-oxidation). The europium-catalyzed aerobic oxidation has a variety of substrate scopes including secondary alcohols and aliphatic alcohols in the optimized condition.[2] The detail mechanistic proposal with condition screening will be discussed during the presentation. We believe that the present europium-catalyzed aerobic oxidation brings new possibility and interest of lanthanide metals to develop redox-cycle based organic transformations in the future.References1 Armelao, L.; Quici, S.; Barigeletti, F.; Accorsi, G.; Bottaro, G.; Cavazzini, M.; Tondello, E. *Coord. Chem. Rev.* **2010**, *254*, 487.2 Kim, S.; Kim, Y.; Jin, H.; Park, M.-H.; Kim, Y. Lee, K.-M.; Kim, M. *Adv. Synth. Catal.* **2019**, *361*, 1259.

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

Oral Presentations for Young Scholars in Organic Division

Room 700A, THU 09:15

Chair: Jun Hee Lee (Dongguk University)

Structural design-promoted tuning of morphological and physical properties in azobenzene-tethered *β*-peptide foldamer

Lianjin Zhang, Hee-Seung Lee[*]

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

The ability to respond to environmental changes is an intrinsic property of living systems. However, the development of synthetic stimuli-responsive molecular systems capable of undergo mechanical work to transform their morphologies and physical properties under external stimuli remains a significant challenge. Here, we report the stimuli-responsive behaviour of azobenzene-tethered *β*-peptide foldamer-based systems using molecular self-assembly approach to find out the structure-property correlation.Systematic investigation of self-assembled structures from rationally designed analogues revealed that the distinct spatial arrangement of chromophore, spacer and foldamer plays pivotal role in determining the morphology and physical properties : graft-foldamer F2, which comprising azobenzene attached to N-terminus of *β*-peptide foldamer via glycine spacer exhibited morphological transformation from plate-like structures to spheres under UV-light and rod-like morphologies under heating condition. Additionally, structural change from plate- or spherical-shape to rod-shape was achieved under heating condition showed phase transition from amorphous to crystalline nature. Accompanied by the morphological transition, strong red fluorescence also emerged during spherical structure formation. The appearance of fluorescence is realized as a synergistic effect of long-lived *cis*-isomer and robust conformational features of *β*-peptide foldamer. These studies emphasize molecular design approach using foldamer for design biocompatible self-assembling micro-architectures that can tune morphologies and functions at macroscale under external stimuli.

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

Oral Presentations for Young Scholars in Organic Division

Room 700A, THU 09:30

Chair: Jun Hee Lee (Dongguk University)

Oppenauer oxidation with allylic aluminum reagents through Cu-catalyzed hydroalumination of allenes

Sangback Lee, SangHyun Lee, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

α-Substituted ketones are very prevalent compounds in organic synthesis and useful intermediates for further chemical transformations. Among numerous methodologies for the synthesis of ketones, selective oxidation of alcohols is a powerful protocol. Although various oxidation methods are available, expensive metal catalysts and difficult-to-handle hazardous reagents are often required. The Oppenauer oxidation of alcohols using a carbonyl compound has known as a highly selective reaction and used simple organic molecules as oxidants and inexpensive mild reagents. In the previous example, metal catalysts such as Mg, Ir, Cr and Ru have been applied for the efficient oxidation. In our study, we developed Oppenauer oxidation of aldehyde with readily prepared allylic aluminum reagents which were generated from the hydroalumination of allene derivatives with diisobutylaluminum hydride(DIBAL-H) in the presence of 5 mol % NHC-CuCl. The oppenauer oxidation with allylic aluminum reagents is an effective and practical strategy to afford the desired α-substituted ketone products in good to high yields.

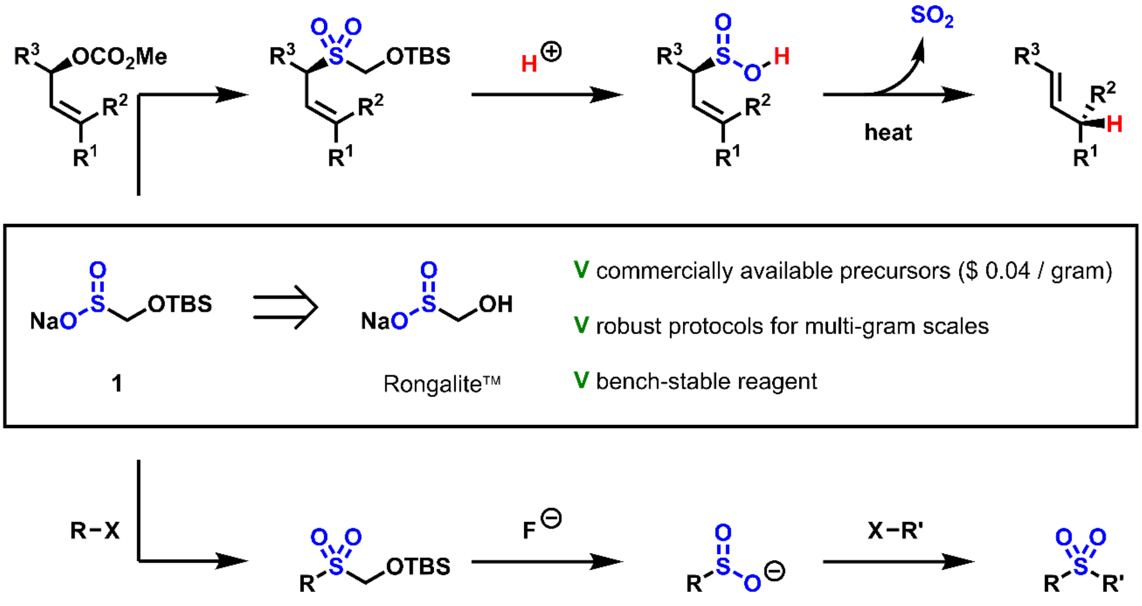
Oral Presentation : **ORGN.O-4**
Oral Presentations for Young Scholars in Organic Division
Room 700A, THU 09:45
Chair: Jun Hee Lee (Dongguk University)

Silyloxymethanesulfinate for Desulfinylation and Sulfonylation

Hyun-Suk Um, Dae-Kwon Kim, Chulbom Lee*

Department of Chemistry, Seoul National University, Korea

Construction of carbon-heteroatom bonds as well as carbon-carbon bonds is of importance in organic synthesis. One of the most well-established synthetic methods is the palladium-catalyzed allylic alkylation, also known as the Tsuji-Trost reaction, which serves as a powerful tool for the regio- and stereoselective allylic substitution. Among numerous variations, the *S*-allylation has highlighted the synthetic versatility of the process, allowing the allylic C-S bond established by Pd catalysis to be used in the subsequent elaborations. Our group has demonstrated that allylic sulfinic acids, derived from the Diels-Alder reaction of 1-sulfenyl ($TBSOCH_2S$) or sulfonyl ($TBSOCH_2SO_2$) dienes, can be targeted as useful intermediates for the synthesis of unusual cyclohexenes. In an effort to further explore this chemistry, we have prepared the novel sulfinate reagent from Rongalite^{TM} for use in the stereoselective allylic reduction, in which allylic carbonates are reduced to the alkene products with high regio- and stereoselectivity through the tandem Tsuji-Trost allylic sulfonation and desulfinyl retro-ene reactions. The potentiality of sulfinate **1** as a sulfur nucleophile has also been manifested with alkyl and aryl electrophiles to forge sulfonyl linkages. Subsequent deprotection of the $TBSOCH_2$ group reveals sulfinates which can be *in situ* coupled with various electrophiles to afford sulfones and sulfonyl derivatives such as sulfonamides and sulfonyl fluorides. The dual reaction mode of sulfinate **1** attests to the protean nature of the reagent for use as a novel reductant and a building block for various sulfonyl structures.


R³ OCO₂Me
R² R¹
OTBS
H⊕
heat
SO₂
H
NaO S OTBS
1
NaO S OH
Rongalite™
V commercially available precursors ($ 0.04 / gram)
V robust protocols for multi-gram scales
V bench-stable reagent
R−X
F⊖
X−R'
R S R'

Oral Presentation : **ORGN.O-5**
Oral Presentations for Young Scholars in Organic Division
Room 700A, THU 10:00
Chair: Jun Hee Lee (Dongguk University)

Cyclosporin O: orally bioavailable cyclic undecapeptide scaffold

Dongjae Lee, Jiwon Seo*

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

In recent 20 years, macrocyclic peptides have tantalized medicinal chemists as a novel type of therapeutics with large surface area and exceptional membrane permeability to regulate intracellular protein-protein interactions (PPIs), one of the challenging targets. Cyclosporin A (CsA) is a representative membrane permeable cyclic peptide, and it tightly binds to an intracellular target, cyclophilin A. Inspired by CsA, diverse cyclic peptide scaffolds with small sizes (6-7 AAs) have been investigated, but they possessed insufficient surface area to involve PPIs. Herein, cyclic undecapeptide scaffold based on cyclosporine O (CsO), a unique member of the cyclosporine family without MeBmt residue, was designed. CsO and its derivatives were synthesized by standard solid-phase peptide synthesis (SPPS) protocol employing the side chain modifications for steric occlusion or on-resin cyclization. NMR spectroscopy and computational modeling based on NMR constraints demonstrated transannular interactions and conformational changes depending on the modified side chains. Passive and cell-based membrane permeability was determined in PAMPA and Caco-2 cell system, respectively, to evaluate the structure-permeability relationship (SPR) study. Pharmacokinetic study for CsO indicated a prominent oral bioavailability considering the size of the molecule. We expect cyclic undecapeptide scaffold based on CsO can be applied as a promising orally bioavailable scaffold to regulate PPIs mediating large surface area.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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

Oral Presentations for Young Scholars in Organic Division

Room 700A, THU 10:15

Chair: Jun Hee Lee (Dongguk University)

Synthesis of Polycyclic Heteroaromatics Doped with Nitrogen

So Jung Kim, Young S. Park*

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

Polycyclic aromatic hydrocarbons (PAHs), containing only carbon and hydrogen atoms, are composed of multiple aromatic rings. These semiconducting carbon-based molecules have been used in organic electronics. The electronic properties of carbon-based materials can be further tuned by incorporating heteroatoms such as nitrogen (N) and phosphorus (P). Tetrabenzo-fused pyracylene (TBP) is one of the cyclopenta-fused PAHs, which includes both tetracene and pyracylene moieties. Interestingly, TBP exhibits an electron-deficient character due to the pyracylene segment. Therefore, additional electrons into the pyracylene moiety by N-doping would change the frontier molecular orbitals of N-doped TBP. Here, we report the synthesis and characterization of N-doped TBP. In this study, we control the position of N atoms through the efficient bottom-up synthetic approaches. In order to elucidate the effect of N-doping, we measure optoelectronic and electrochemical properties of our molecule. Currently, further studies on PN-doped PAHs are in progress in our laboratory. **References**1. M. Stepien *et al.*, *Chem. Rev.* **2017**, *117*, 3479–3716.2. Chaolumen *et al.*, *Angew. Chem. Int. Ed.* **2015**, *54*, 9308–9312.

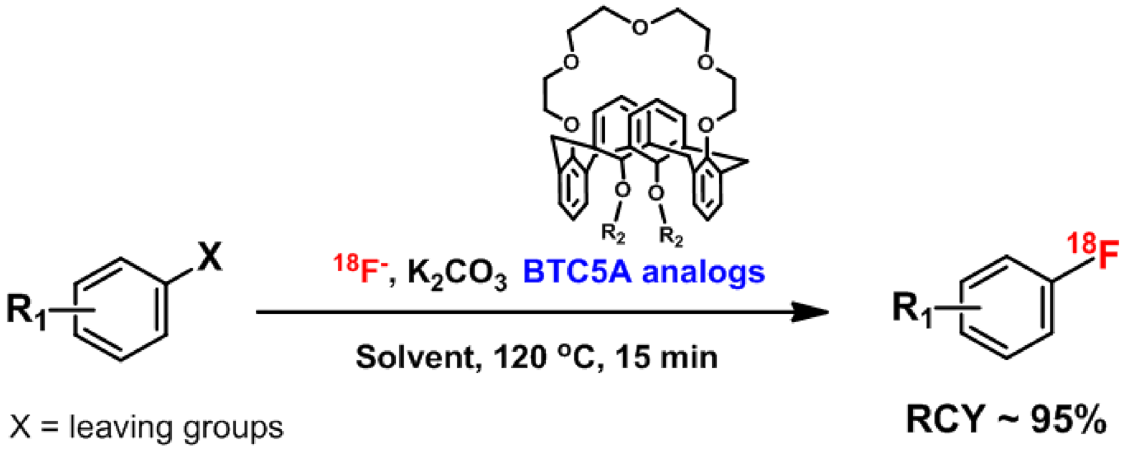
Oral Presentation : **ORGN.O-7**
Oral Presentations for Young Scholars in Organic Division
Room 700A, THU 10:30
Chair: Jun Hee Lee (Dongguk University)

BTC5A (Bis-Triethylene glycol-functionalized Crown-5-calix[4]Arene) analogs as a new phase-transfer catalysts for nucleophilic aromatic ^{18}F-fluorination

Wonchang Lee, Byung Chul Lee[1,*], Dong Wook Kim[2]

Seoul National University, Korea
[1]*Department of Nuclear Medicine, Seoul National University Bundang Hospital, Korea*
[2]*Department of Chemistry, Inha University, Korea*

Fluorine-18 has been used predominantly as a useful positron emitting isotope to prepare the radiotracer in the application of positron emission tomography (PET). In particular, introduction of fluorine-18 into aromatic system is more required to avoid the metabolic defluorination of radiotracer by the reason of a high in vivo stability of a C_{Ar}-F bond. Herein, we intend to evaluate an effective aromatic ^{18}F-fluorination in various conditions by using BTC5A analogs as a new phase transfer catalyst (PTC).To optimize the fluorine incorporation condition, the reactivity of PTC (BTC5A analogs or Kryptofix2.2.2 ($K_{2.2.2}$)) was investigated in various solvents, temperatures, fluorine sources, amounts of bases, and two diaryliodonium salt precursors. In the stability test of precursors in the presence of PTC and base except the fluorine source, the BTC5A treated group showed up to 30% higher stability of the precursor than that of the $K_{2.2.2}$ treated group. When using TEMPO as radical scavenger, we found that precursor was more stable in basic conditions. The optimized aromatic fluorination from the precursor by using BTC5A analogs showed the highest yields up to 80%, which is 10 times higher than that by using $K_{2.2.2}$. In ^{18}F-labeling experiments, aromatic ^{18}F-fluorination by using BTC5A analogs showed up to 82%, which is 3 times higher than that that by using $K_{2.2.2}$. Especially, the well-known aromatic ^{18}F-labeled radiopharmaceutical, [^{18}F]Flumazenil was prepared in 95% radiochemical yield by using BTC5A analogs, which is 2 times higher than that of followed the reported method.In this study, we successfully developed the enhanced aromatic ^{18}F-fluorination with a new type of PTC, BTC5A analog which is superior to the general PTC ($K_{2.2.2}$). This BTC5A analog can serve as a facile and efficient tool for the development of radiopharmaceuticals.



X = leaving groups

R_1 = various functional groups

R_2 = H, $(CH_2CH_2O)_2CH_2CH_2OH$, or $(CH_2CH_2O)_2CH_2CH_2OCH_3$

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

Oral Presentations for Young Scholars in Organic Division

Room 700A, THU 10:45

Chair: Jun Hee Lee (Dongguk University)

Lewis Acid-Catalyzed Synthesis of Organophosphine Oxides via Hydrophosphinylation of *N*-Heteroaryl-Substituted Alkenes

Jimin Han, Jongwon Kim, Yunmi Lee*

Department of Chemistry, Yonsei University, Korea

Organophosphorus compounds are valuable building blocks, which are widely applied in fields of organic synthesis, pharmaceuticals, agrochemicals and material science. Indeed, the functionalized phosphines have attracted growing attention because of their potential roles as versatile phosphine ligands in developing transition-metal catalysis. Among various synthetic methods to prepare organophosphorus compounds, hydrophosphinylation, the addition reaction of phosphorus-hydrogen bond across the unsaturated moiety, is the atom-economical process that incorporates phosphorus atom to diverse range of organic compounds. In particular, hydrophosphinylation of alkenes is one of the classic and practical routes to synthesize various organophosphorus compounds, owing to the versatility and accessibility of alkene substrates. In this talk, we describe the boron-catalyzed hydrophosphinylation of multisubstituted alkenes that possess *N*-heteroarene as one of the substituents, thereby generating a series of highly substituted phosphorus and nitrogen containing organophosphorus compounds. Specifically, inexpensive and commercially available boron trifluoride diethyl etherate (BF_3•Et_2O) catalyzes the addition of diaryl phosphine oxides to alkenes under mild conditions in good to excellent yields. This easily operative protocol is an efficient strategy to install various aromatic *N*-heterocycles on secondary phosphine oxides. Furthermore, such phosphorus and nitrogen containing compounds are valuable because of their potential roles as P,N-bidentate ligands.

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

Oral Presentation of Young Discovery Chemists

Room 607, THU 09:00

Chair: Sang Min Lim (KIST)

Water-Soluble Organic Nanoparticles for Biocompatible Photodynamic Therapy In Vitro and In Vivo

Il Yoon

PDT Laboratory, Inje University, Korea

Photodynamic therapy (PDT) is a promising cancer therapy with non-invasive treatment without side-effect. Photosensitizers (PSs) used in PDT are usually hydrophobic, and therefore those are not water-soluble. Water-soluble PSs are rare in PDT research. Therefore, it is a great challenge to prepare water-soluble PS for clinical trials in PDT. Here we prepared water-soluble organic nanoparticles (WSON) by very simple and easy preparation method. WSON were made in nanometer size with good water-solubility as well as high water stability. We evaluated intracellular accumulation and cell viability of those WSONs and PEG-WSONs. Free PSs and PEG-WSONs displayed a good PDT activity in vitro and in vivo. This result is important not only to prepare WSON using hydrophobic PS as water-soluble PS having high water stability in nanometer size but also to enhance PDT activity with reduced dark toxicity suitable for clinical trials in PDT.

Oral Presentation : **MEDI.O-2**
Oral Presentation of Young Discovery Chemists
Room 607, THU 09:15
Chair: Sang Min Lim (KIST)

Targeted Protein Degradation via the N-End Rule Pathway

Yeongju Lee, Hyun-Suk Lim*

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

PROteloysis TArgeting Chimera (PROTAC) technology has emerged as a therapeutic strategy to degrade proteins related to diseases. However, developed PROTAC molecules only target a limited number of E3 ligases, thereby being applicable to specific cell lines that express PROTAC targeted E3 ligases. To be widely applicable in various cell lines, we designed a new concept of heterobifunctional degraders using N-end rule pathway without identification of new E3 ligases and selective ligands of the identified E3 ligases. The new degradation system couples N-degrons, which are degradation signals (degrons) in protein N-terminus, with the ligands of target proteins. To demonstrate feasibility of our strategy, we conjugated N-degrons to the previously reported cell-permeable stapled peptide **yl-2**[1] to be recognized as degradation signals resulting in ubiquitination and degradation of target protein NCOA1. We successfully demonstrated that the resultant compound exhibited proteasome-dependent degradation of NCOA1 while PROTAC molecules had no degradation effect. Furthermore, we examined that the designed compound depleted NCOA1 inducing the repression of breast cancer cells migration and invasion *in vitro* and *in vivo*. This new concept of chemical degraders will serve a widely applicable degradation method for targeting disease-related proteins and provide a strategy for new therapeutics.Reference[1] Lee, Y.; Yoon, H.; Hwang, S. M.; Shin, M. K.; Lee, J. H.; Oh, M.; Im, S. H.; Song, J.; Lim, H. S.; “Targeted Inhibition of the NCOA1/STAT6 Protein-Protein Interaction” *J. Am. Chem. Soc.* **2017**, *139*, 16056

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

Oral Presentation of Young Discovery Chemists

Room 607, THU 09:30

Chair: Sang Min Lim (KIST)

Discovery of Novel β-arrestin-biased S1P1 Agonists for Treatment of Multiple Sclerosis

WooSeung Son, Hyeon Jeong Kim[1], Siwon Kim[2], Jong-Hyun Park[3], Sang Min Lim[2], Ki Duk Park[1], Kyu-Sung Jeong, Ae Nim Pae[2,*]

Department of Chemistry, Yonsei University, Korea
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*
[2]*Korea Institute of Science and Technology, Korea*
[3]*Convergence Research Center for Dementia DTC, Korea Institute of Science and Technology, Korea*

Multiple sclerosis (MS) is a chronic, progressive autoimmune disease which causes demyelination of the CNS. The non-selective Sphingosine-1-phosphate (S1P) receptor modulator, FTY720, binds to S1P1, 3, 4, 5. In Human clinical trials, it is associated with diverse side effects such as hypertension by S1P3 agonism. 1 Our rationale of developing novel selective S1P1 receptor Agonist is to be lower the circulating lymphocytes more efficiently by internalization of S1P1 on lymphocyte. 2 We designed and synthesized S1P1 receptor agonists with selectivity against S1P3 receptor via in silico docking study on S1P1 receptor crystal structure. The synthesized compound KKPS0075 showed remarkable in vitro activities (Ca2+ signaling assay, EC50=23 nM, β-arrestin assay, EC50=1.98 nM and Internalization assay, EC50=0.65 nM) with sparing activity against S1P3 receptor. Furthermore, the compound KKPS0073 show β-arrestin biased signaling as S1P1 agonist(Ca2+ signaling assay, EC50=111 nM, β-arrestin assay, EC50=0.17 nM and Internalization assay, EC50=5.04 nM). Optimization of pharmacokinetic properties and in vivo study is ongoing.

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

Oral Presentation of Young Discovery Chemists

Room 607, THU 09:45

Chair: Sang Min Lim (KIST)

Hydrogel Fibers Network for Three-Dimensional Cell Cultures

Sungrok Wang, Myung-Han Yoon*

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

In biomedical engineering, electrospun fibers have been extensively used as porous scaffolds for a variety of three-dimensional (3-D) cell cultures however there still are practical issues such as low optical transparency, unfavorable mechanical stiffness, poor dimension controllability, etc. Herein, we fabricated hydrogel fiber suspension with zwitterionic properties by grinding electrospun fibers. The resultant suspension of hydrogel fibers exhibited excellent biodegradability, high optical transparency, controllable mechanical properties, and stable dispersion in water. When the oppositely charged fiber suspensions were mixed together, the hydrogel fibers were entangled forming hydrogel fibers network with microscale porosity. Finally, the entangle fibers can act as 3-D cell culture scaffold and, it was demonstrated that stiffness, overall diameter, and swelling ratio of hydrogel fibers can be easily modulated to optimize for various applications.

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

Oral Presentation of Young Discovery Chemists

Room 607, THU 10:00

Chair: Sang Min Lim (KIST)

Identification of new human targets of antibiotics toward drug repositioning

Sung Min Cho, Ho Jeong Kwon[1,*]

Biotechnology, Yonsei University, Korea

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

Drug repositioning saves the time and cost of drug development in difficulties of FDA approval. It is a promising approach reducing risk of side effects because it is already approved drugs. In this study, reverse chemical proteomics enables access to new targets and pathways of existing drugs targeting anti-infectious disases. Here are two case compounds of Artesunate (ART) and Daptomycin (DAP). Both ART and DAP are the most potent and safe antimalarial and antibacterial drugs, respectively. Despite their clinical potential, no human target for them are known. The unbiased interrogation of several human cDNA libraries, displayed on bacteriophage T7, revealed a high affinity human target of them; the Bcl-2 antagonist of cell death promoter (BAD) and ribosomal protein S19 (RPS19), respectively. ART inhibits the phosphorylation of BAD, promoting the formation of the BAD/Bcl-xL complex and the subsequent intrinsic apoptosis. In addition, DAP exhibits selective growth inhibition of some cell lines, particularly MCF7 and HUVECs. This ability of DAP is due to regulate the expression of cell growth related cytokines such as VEGF and EGF, resulting in suppressed tumour invasion. Collectively, these two case studies of reverse chemical proteomics demonstrate the potential of drug repositioning of antibiotics to anticancer drugs.

Oral Presentation : **MEDI.O-6**
Oral Presentation of Young Discovery Chemists
Room 607, THU 10:15
Chair: Sang Min Lim (KIST)

Rh(III)-Catalyzed Synthesis of N-heterocyclic compounds and its application to bioimaging agent

Sangbong Lee, Ye Ri Han, Jungwook Chin, Su-Jeong Lee, Minseon Jeong, Sung Jin Cho[*], Dong-Su Kim[*]

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

Synthesis of N-heterocylic compounds using Rh(III) catalysis received great attentions in various fields of studies such as pharmaceutical and materials area. Recently, we developed synthetic methods for the synthesis of N-heterocyclic salt compounds using Rh(III)/Cu(II) complex. Interestingly, we found that their fluorescent spectra showed over the full color region. Based on these previous studies, we attempted for application of fluorescent materials to diagnostic bioimaging in vivo model. For successful application of fluorescent materials as imaging agent, several in vitro and in vivo experiments were performed. As a result, we found that benzoquinolizinium salt may serve as an in vivo imaging agent for detection of inflamed lesions. This result can be applied to the diagnosis of disease.

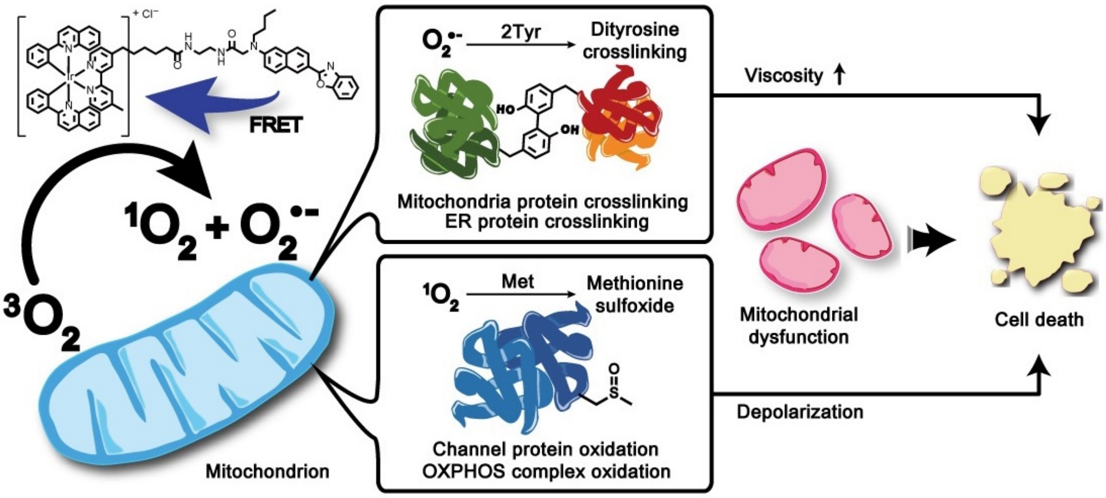
Oral Presentation : **MEDI.O-7**
Oral Presentation of Young Discovery Chemists
Room 607, THU 10:30
Chair: Sang Min Lim (KIST)

Monitoring Mitochondrial Response to Oxidative Stress via an Intramolecular Energy Transfer-based Iridium(III) Photosensitizer

Chaiheon Lee, Jung Seung Nam, Tae-Hyuk Kwon*

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

Elucidating the process of oxidation-mediated cell death is one of the important challenges in photodynamic therapy (PDT). The key component of PDT is a photosensitizer which give cancer cells strong oxidative stress inducing protein dysfunctions through reactive oxygen species (ROS) production. A mitochondrion, a sensitive subcellular structure to oxidative stress, is involved in cellular energy production and initiation of apoptosis. Recently, developing photosensitizers targeting mitochondria has recently been recognized as an efficient strategy for PDT. However, it has been veiled what proteins are damaged when instantaneous oxidative stress occurs. Furthermore, various phenomena in mitochondria (i.e. change in mitochondrial microenvironment) resulting from the protein dysfunction have not been fully investigated even though they are deeply involved in initiation of cell death. The organometallic iridium(III) complexes exhibit proper characteristics to monitor and analysis the effect of photosensitizers on mitochondria. Thus, we newly synthesized strong photosensitizer, **Ir-OA**, targeting mitochondria. The energy transfer-based molecular design strategy with an energy donor of **Ir-OA** provides acceleration of ROS production. Hence, we successfully utilized **Ir-OA** for (i) efficient mitochondria-target PDT, (ii) monitoring change in mitochondrial microenvironment (i.e. viscosity, polarity, and morphology) in response to oxidative stress, and (iii) profiling the damaged proteins by oxidative stress. Finally, we established a reasonable overall mechanistic pathway how the photosensitizers affect mitochondria and cause effective cell death, corroborating correlation between mitochondrial microenvironment change and damaged proteome.


+ Cl⁻
FRET
$^1O_2 + O_2^{\bullet-}$
$^3O_2$
Mitochondrion
$O_2^{\bullet-}$
2Tyr
Dityrosine crosslinking
HO
OH
Mitochondria protein crosslinking
ER protein crosslinking
$^1O_2$
Met
Methionine sulfoxide
Channel protein oxidation
OXPHOS complex oxidation
Viscosity ↑
Mitochondrial dysfunction
Depolarization
Cell death

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

Oral Presentation of Young Discovery Chemists

Room 607, THU 10:45

Chair: Sang Min Lim (KIST)

Total Synthesis of Biemamide B and D from chiral Aziridine

Nikhil Srivastava, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, India

First facile asymmetric synthesis of both enantiomers of 5,6-dihydrouracil-type marine natural products biemamide B and D as potential TGF-β inhibitors from enantiopure aziridine-2-carboxylate. We established the short, efficient and expedite synthetic route which involves regio- and stereoselective aziridine ring opening via azide and construction of 5,6-dihydrouracil core with the formation of C-N bond by base-induced intramolecular cyclization reaction as key steps.

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

Oral Presentation for Young Material Chemists

Room 700B, THU 09:00

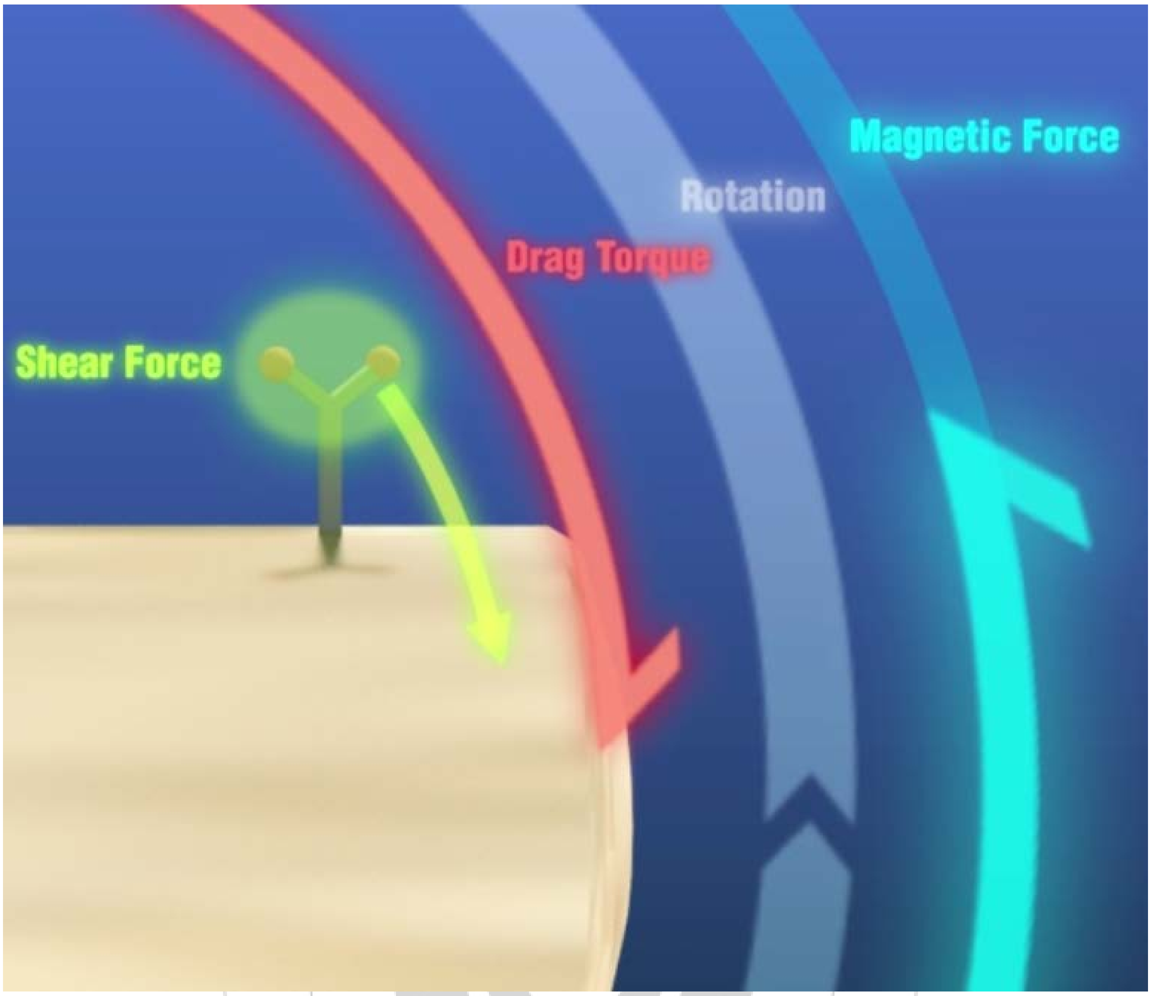
Chair: Kwang Seob Jeong (Korea University)

Plasmonic Nanodisks Embedded in Magnetic Gyro-Nanorods for Fourier Transform Surface Plasmon Resonance Based Biosensing

Seongkeun Ih, Jieun Shin, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

Herein, we demonstrated a simple and effective LSPR based biosensing with magnetic rotation by inserted ferromagnetic segment into plasmonic blocks. As template-based electrochemical deposition method enabled to act as plasmonic nanoparticle with magnetic functionality. Due to the presence of the magnetic segment, the synthesized gyro-nanodisks (GNDs) are not only plasmonically active, but are also magnetically response. Owing to the magnetically-responsive and plasmonically-active GNDs, periodic extinction signals were generated under the external rotating magnetic field, which can be converted to frequency-domains using Fourier-transform. After binding a target molecule on GNDs, an increase in the resistance force causes a dynamically perturbed frequency signal which allows us to investigate biodetection. By modulating the design of the GNDs with respect to number and the embedded location of plasmonic nanodisks, we investigated the correlation between hydrodynamic force and the magnetic cancellation effect. The concepts and approaches will contribute to further advanced sensing module performance, as well as a better understanding of dynamic nanoparticle system, by modulated periodic fluctuation of surface plasmon bands under the external magnetic fields.


Magnetic Force
Rotation
Drag Torque
Shear Force

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

Oral Presentation for Young Material Chemists

Room 700B, THU 09:15

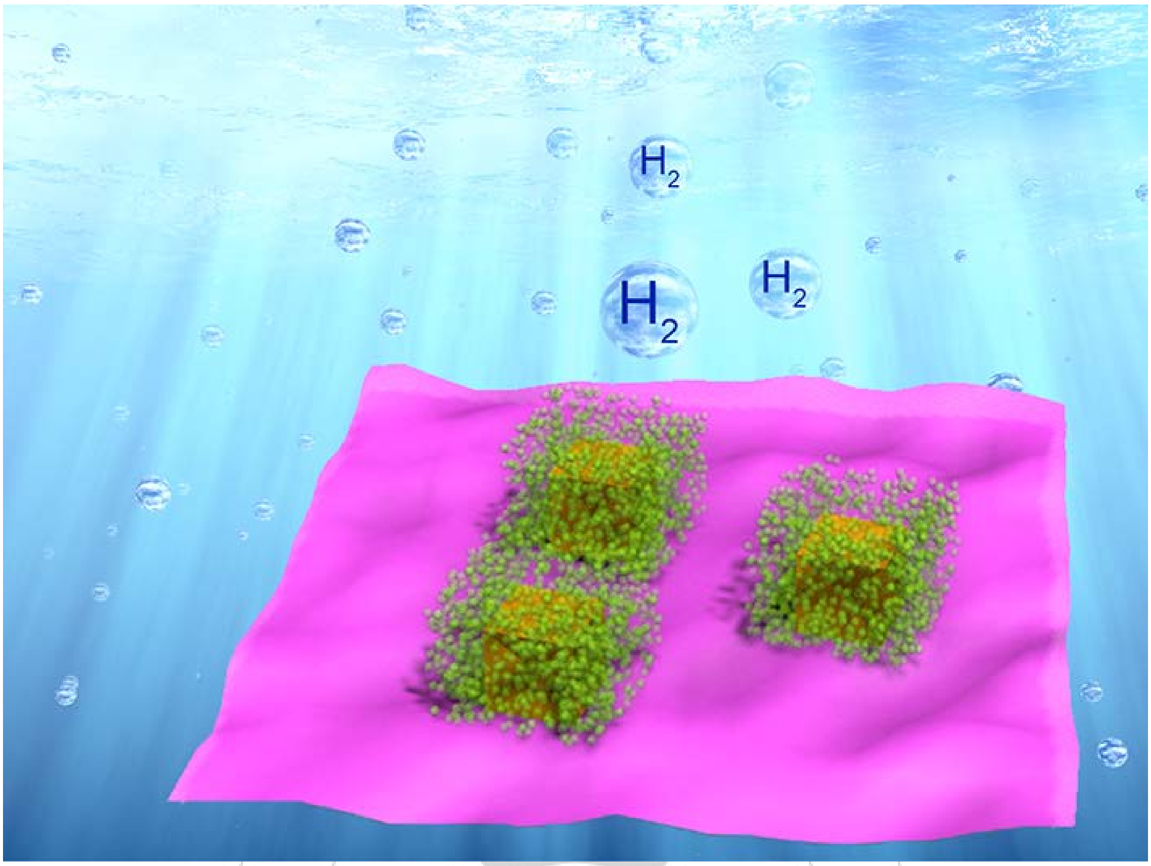
Chair: Kwang Seob Jeong (Korea University)

Plasmonic Metal-Semiconductor Ternary Hybrid Nanostructures for Efficient Visible-Light Photocatalysis

Dae Han Wi, Jong Wook Hong[1], Sang Woo Han*

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

Solar-driven production of chemical fuels through photocatalysis holds great promise for addressing the ever-increasing energy and environmental issues. However, its practical application is limited due to low light harvesting efficiency, fast charge recombination, and low stability of current photocatalysts. Here, we introduce a high-performance solar energy conversion platform constructed by the intimate coupling of two different complementary semiconductors (MoS_2 and CdS) and morphology-controlled plasmonic metal nanocrystals (concave cubic Au nanocrystals) in a controlled manner. The sequential Au nanocrystal anchoring and CdS growth on two-dimensional exfoliated MoS_2 nanosheets successfully yielded intimately coupled plasmonic metal–semiconductor ternary hybrids. The prepared hybrid photocatalysts exhibited superb hydrogen evolution capability under visible-light irradiation, which can be attributed to the synergistic integration of the advantages of semiconductor–semiconductor coupling, such as the broadening of light absorption and the retardation of charge recombination, and plasmon energy transfer from Au nanocrystals to semiconductors via the hot electron transfer mechanism.


H2
H2
H2

Oral Presentation : **MAT.O-3**
Oral Presentation for Young Material Chemists
Room 700B, THU 09:30
Chair: Kwang Seob Jeong (Korea University)

AIPE Active Deep-Red to Near-Infrared Phosphorescence from Iridium(III) Complexes for Solution Processable PhOLEDs

Hae Un Kim, Seung Un Ryu, Sungjin Park, Seyeong Lim, Taehyun Kim, Taiho Park*

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

Studies of materials and devices that emit near-infrared (NIR-) wavelengths have been carried out in various fields. However, it is still a difficult task to develop luminous materials that have an efficient, stable and low-cost NIR luminescence. Herein, a series of complex molecules have been developed for NIR emission to investigate the effects of electron-withdrawing and -donating substituents fixed to the quinoline moiety of (benzo[*b*]thiophen-2-yl)quinoline cyclometalating ligands. In the excited state of solution, powder, doped polymer film and frozen matrix state, a photophysical study was carried out to investigate the substitution effect. The $–C_6H_5$ and $–CF_3$ substituted complexes showed high phosphorescence quantum efficiency with aggregation-induced phosphorescence emission (AIPE). The device fabricated by solution-processable method showed maximum external quantum efficiency (EQE) value of 7.29%.

Oral Presentation : **MAT.O-4**
Oral Presentation for Young Material Chemists
Room 700B, THU 09:45
Chair: Kwang Seob Jeong (Korea University)

Controlling Polymorphism of Polymer-Coated Nanocrystal Superlattices

Hongseok Yun, Bumjoon Kim[1,*]

Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemical Engineering & Biotechnology, Korea Advanced Institute of Science and Technology, Korea*

Self-assembly of colloidal nanocrystals is an effective route to build novel materials that cannot be achieved by conventional techniques. Here, I will present the control of the packing symmetry of polystyrene-coated Au nanoparticles (Au@PS NPs) by controlling grafting density, molecular weight (Mn) of PS, and diameter of Au NPs. I will discuss the factors that determine the packing symmetry of polymer-coated nanocrystals. Finally, I will demonstrate the theoretical prediction of interparticle distance and packing symmetry of 3-dimensionally packed nanocrystal superlattices by applying "effective softness" of NPs to optimal packing model. This work demonstrates effective ways to manipulate the self-assembly behavior of polymer-coated nanocrystals, which is very important for the fabrication of potential NP-based devices.

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

Oral Presentation for Young Material Chemists

Room 700B, THU 10:00

Chair: Kwang Seob Jeong (Korea University)

Considering Critical Factors of Advanced Anode Material for High Performance Lithium-Ion Batteries

Minseong Ko

Pukyong National University, Korea

While existing carbonaceous anodes are approaching a practical limit, silicon (Si) has been vigorously examined as a potential alternative due to its exceptional gravimetric capacity (3579 mAh/g) and abundance. However, the actual implementation of Si anodes has been still impeded by their difficulties in the electrode calendaring and the requirement for excessive binder and conductive agent, arising from the brittleness, large volume expansion (> 300%) and low electrical conductivity (1.56×10^{-3} S/m). Considering the rational approach to using silicon in high-energy LIBs, the Si-based materials mixed with graphite has been re-illuminated as a feasible alternative as next-generation anodes. Here, I would like to demonstrate a silicon nanolayer-embedded graphite (SGC) hybrid and performed detailed one-to-one comparisons with industrially developed benchmarking samples under the industrial electrode density (> 1.6 g/cc), areal capacity (> 3 mAh/cm2), and a small amount of binder (3 wt%) in a slurry. Comparing to the benchmarking samples, SGC was successful in preserving electrode integrity from volume variation, and exhibited 92% of high 1st cycle coulombic efficiency (CE) and rapid increase of cycling CE greater than 99.5% after 6th cycle. As a result, even in full-cell, SGC allowed a higher cell capacity (3.02mAh/cm2) at the first formation cycle and more stable cycling behavior than benchmarking samples. Overall, the favorable compatibility between SGC and conventional graphite has presented great potential for practicable high-energy LIBs anode.

Oral Presentation : **MAT.O-6**
Oral Presentation for Young Material Chemists
Room 700B, THU 10:20
Chair: Kwang Seob Jeong (Korea University)

Anisotropic Plasmonic Nanoparticle Self-Assembly in Liquids

Juyeong Kim

Chemistry, Gyeongsang National University, Korea

The solution phase dominates chemistry, serving as host for processes ranging in organic syntheses, colloidal nanoparticle formation, catalysis, and self-assembly. The liquid-phase transmission electron microscopy (TEM), an emerging in situ imaging tool, allows direct imaging of nanoscale materials in solution with high spatiotemporal resolution, also providing different liquid environment and electrochemical control. Thus, imaging solution-phase nanoscale events gain unique information for fundamental questions in chemical processes.We use liquid-phase TEM to watch self-assembly of gold triangular prisms and investigate the assembly dynamics. The in situ monitoring, single nanoparticle tracking, and the marked conceptual similarity between molecular reactions and nanoparticle self-assembly combined elucidate the following mechanistic understanding: a step-growth polymerization based assembly statistics, kinetic pathways sampling particle curvature dependent energy minima and their interconversions, and directed assembly into polymorphs (linear or cyclic chains) through in situ modulation of the prism bonding geometry. Our study bridges the constituent kinetics on the molecular and nanoparticle length scales, which enriches the design rules in directed self-assembly of anisotropic plasmonic nanoparticles.

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

Oral Presentation for Young Material Chemists

Room 700B, THU 10:40

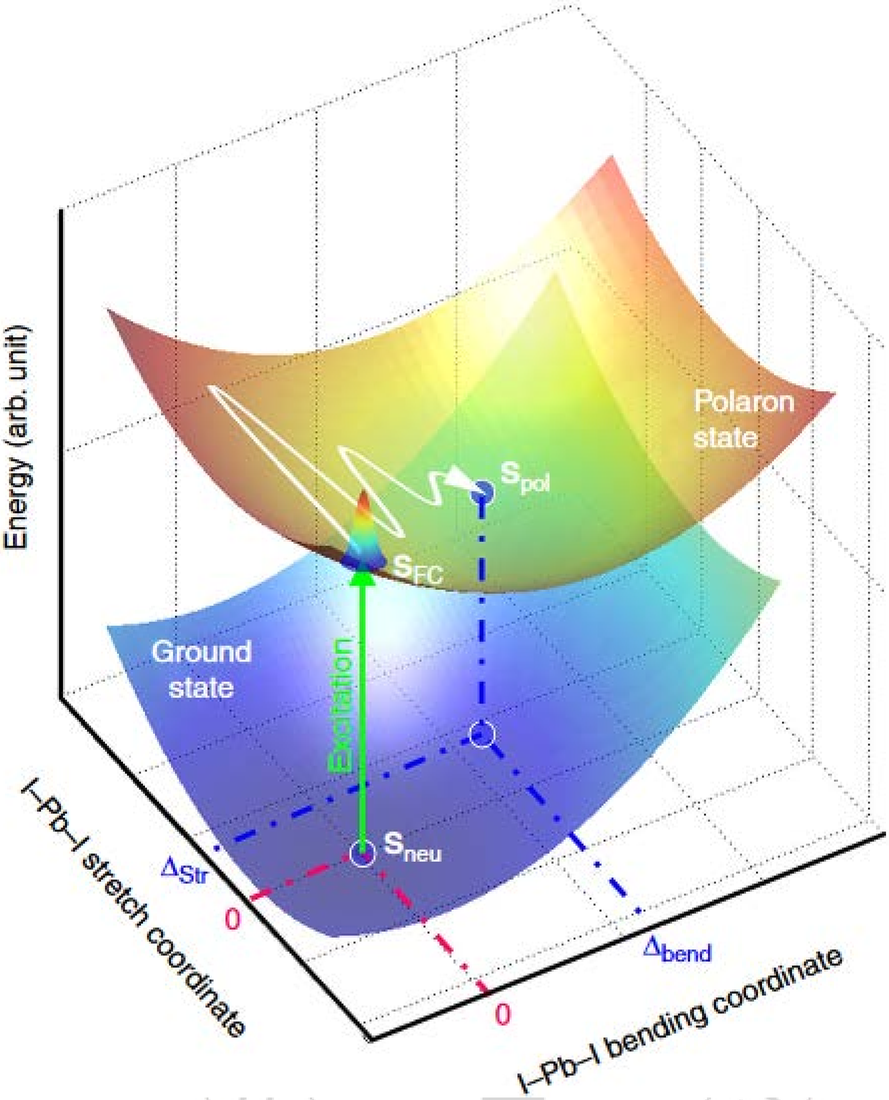
Chair: Kwang Seob Jeong (Korea University)

Excited-State Polaron Formation Dynamics of Hybrid Organic-Inorganic Perovskites

Myeongkee Park

Department of Chemistry, Dong-A University, Korea

The formation of a polaron, a charged quasi-particle, may account for the high power conversion efficiency (~25 %) achieved in hybrid organic-inorganic perovskite solar cells. In according to polaron screening effect hypothesis, the electric dipole reorientations of the organic cations and the structural distortions of the inorganic frameworks are the key factors to have a long-lived polaronic excited state associated with high power conversion efficiencies. This also implies that hybrid organic-inorganic perovskites have different energy minima between the neutral ground state and polaronic excited-state potential energy surfaces along with polaron formation coordinates. However, most of the studies on the polaron are based on theoretical results, and a few experimental results have shown excited-state structural changes. Thus, it is necessary to have more experimental evidence to disclose polaron structures and formation dynamics. Recently, we have studied coherent nuclear wave packets of Pb-I framework (oscillating at $^{-1}$) employing femtosecond transient absorption spectroscopy and first-principles density functional theory. Our results clearly present the experimental evidence on the structural displacements between the ground and excited states. In addition, we have found that these wave packets turn to be correlated to the polaron formation dynamics.


Energy (arb. unit)
Polaron state
S_pol
S_FC
Excitation
Ground state
S_neu
Δ_Str
0
I–Pb–I stretch coordinate
Δ_bend
0
I–Pb–I bending coordinate

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 10:30

Chair: Sang-Il Choi (Kyungpook National University)

Getting Wonderfully Lost in Electrochemistry; From Old Sites of electrochemistry To Popular Attractions

Seongpil Hwang

Department of Advanced Materials Chemistry, Korea University, Korea

Recently electrochemistry have been drawn much interest since our society requires the innovation both in energy and biotechnology. Lots of scientists and engineers visit, live and explore the attractive districts and suburbs of electrochemistry; electrodics, ionics, energy, sensors, and so on. In this symposium, I want to share my exploration as a local in the city of electrochemisty with audience. Itinerary of this seminar will range from the nature of electrons to trending places of solar fuel and electronic skins. Don’t forget historical sites of electrodics and ionics, too. Hope to enjoy this seminar and to share the inspiration on electrochemistry with each other.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 09:00

Chair: Sang-Il Choi (Kyungpook National University)

Enhanced Electrocatalytic Performance of Fe@Pt Core-Shell Nanoparticles for Cathode of PEMFC

Ah-Hyeon Park, Young-Uk Kwon*

Department of Chemistry, Sungkyunkwan University, Korea

As renewable energy conversion and storage system is one of the main challenges, a fuel cell electric vehicle (FCEV) is developed to solve pollution from CO_2 emission and oil depletion issues. According to this, the low-platinum nanoparticle has been studied to replace precious metal catalysts used in metal-air batteries and fuel cells. Ultrasound-assisted polyol synthesis (UPS) is a method that uses ultrasonic energy to produce small and uniform size core-shell nanoparticles on support with even distribution. Platinum(Ⅱ) acetylacetonate and Iron(Ⅲ) acetylacetonate as a metal precursor and carbon support were dispersed in ethylene glycol which is reducing agent and irradiated by ultrasound for 3 h to reduce to the metal nanoparticles, followed by washing and drying to obtain a powder. The structural properties of catalysts synthesized by the sonochemical method are strongly dependent on the source of metal, carbon support, chemical properties of the solvent, a temperature of the solution, energy of sonicator, and after-treatment processes such as acid treatment or calcination and affect catalytic activity and stability. The characterization caused by synthesis variable was observed by analysis that solution color visualization, X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscope (TEM), inductively coupled plasma atomic emission spectroscopy (ICP-AES) and electrocatalytic performance. Our synthesized electrocatalysts show improved electrochemically active surface area (ECSA) and ORR catalytic activity and durability compared to commercial Platinum and this method can apply to the mass production of electrocatalyst with activity corresponding to the commercial catalyst as controlling the variable of UPS.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 09:10

Chair: Sang-Il Choi (Kyungpook National University)

Wide-temperature operation of lithium metal batteries enabled by localized high-concentration electrolytes

Kisung Park, Hochun Lee*

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

The success of rechargeable Li metal batteries (LMBs) hinges on the ability of suitable electrolytes to enable high Li cycling Coulombic efficiency without dendrite formation. Recently, to address the aforementioned issues, localized high-concentration electrolytes (LHCEs) employing a non-coordinating fluorinated ether were introduced. However, very little is known about the performance of LHCEs under harsh temperature conditions. Herein, we investigate glyme-based LHCE (gLHCE) over a wide temperature range (5−60 °C) with a focus on the beneficial role of the fluorinated ether. Compared to glyme-based high-concentration electrolyte (gHCE), gLHCE displays improved physicochemical properties, good wettability toward polyethylene separators, and non-flammability due to the advantageous character of the fluorinated ether. In-depth analysis confirms that in gLHCE, most FSI-anions exist as contact ion pairs and agglomerates, leading to an inorganic-rich solid electrolyte interphase on the Li anode that mitigates the side reactions with the electrolyte and facilitates the interfacial charge transport. The formidable advantages of gLHCE enable an excellent Li cycling behavior and long-term stability of FeS_2/Li and anode-free $LiFePO_4$/Cu cells over 5−60 °C. This work demonstrates unexplored advantages of LHCEs as promising LMB electrolytes and elucidates the underlying mechanism of the beneficial role of the fluorinated ether.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 09:20

Chair: Sang-Il Choi (Kyungpook National University)

Development of Covalent Organic Frameworks-based Lithium-ion Batteries using Azo moiety

Vikram Singh, **Hye Ryung Byon**[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

We demonstrate a positive organic electrode of covalent organic framework (COF) integrated with redox-active azo-moiety. The COF is a promising molecular building block to provide porous ionic channel, suppressed solubility, and feasible design of three-dimensional structure. We introduced redox-active azo-moiety (N=N) through various molecular linkages to COF to control conjugated characteristics and chemical stability. The optimum AZO-integrated COFs had well-established crystal structure and superior stability, delivering 120 mAh g–1 specific capacity (Q_{COF}) at 1 C in 1.2–2.6 V range. This Li-ion battery also displayed stable 5000 cycles at 10 C and high rate capability up to 40 C. Further, directed growth of few COF layers on carbon nanotubes improved total electrode conductivity and Li^+ mobility, evidenced by a 20% increase in capacity at 1 C. In-situ Raman spectroscopy revealed the participation of N=N, C-S and π_{ring} to the reversible electrochemical process. In the presentation, I will also discuss the role of molecular linkages in AZO-based COF and its effect for battery performance in detail.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 09:30

Chair: Sang-Il Choi (Kyungpook National University)

Over a 16% Solar-to-CO Conversion from Dilute CO_2 Streams Catalyzed by Gold Nanoclusters Exhibiting a High CO_2 Binding Affinity

Hoeun Seong, **Dongil Lee***

Department of Chemistry, Yonsei University, Korea

Development of efficient and selective electrocatalysts is a key challenge to achieve an industry-relevant electrochemical CO2 reduction reaction (CO2RR) to produce commodity chemicals. Here, we report that Au25 clusters with Au-thiolate staple motifs can electrocatalyze CO2 to CO without energy loss and achieve a high CO2RR current density of 540 mA cm-2 in a gas phase reactor. An electrochemical kinetic investigation revealed that the excellent CO2RR activity of the Au25 originates from a strong CO2 binding affinity which also leads to improved CO2 electrolysis performance in a dilute CO2 stream. Finally, we constructed a solar driven CO2 electrolysis device by powering a Au25 electrolyzer (EZ) with a Ga0.5In0.5P/GaAs photovoltaic (PV) cell and achieved an 18.0% efficient solar to CO conversion (STC) efficiency for 12 hours. In addition, our integrated Au25 PV-EZ has an exceptional 15.9% STC efficiency and an ~10% solar driven single path CO2 conversion rate in a 10% CO2 gas stream, i.e., a typical CO2 concentration in a flue gas, due to the excellent catalytic property of the Au25 clusters at a low overpotential and low CO2 partial pressure.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 09:40

Chair: Sang-Il Choi (Kyungpook National University)

Synthesis of Nanoscale Pt(100) Surface Decorated with $Ni(OH)_2$ for Alkaline Hydrogen Evolution Reaction

Youngmin Hong, Sang-Il Choi*

Department of Chemistry, Kyungpook National University, Korea

The hydrogen evolution reaction (HER) is a key step in many industrial processes, including water electrolysis, metal deposition, and fuel production from CO_2 reduction. In particular, the production of H_2 through the HER in water electrolyzers has recently received large attention due to the increasing demand for H_2 gas as a key energy source for renewable energy systems. Recently, Subbaraman and co-workers demonstrated that the $Ni(OH)_2$ clusters electrochemically deposited on a Pt(111) electrode could significantly enhance the HER in an alkaline medium due to a bifunctional mode. Specifically, the edges of oxophilic $Ni(OH)_2$ clusters promote the dissociation of water and concomitant generation of H_{ad} that subsequently adsorbs on nearby Pt surfaces and finally recombines into molecular hydrogen (H_2). This bifunctional approach presents a promising strategy for enhancing HER activity in an alkaline electrolyte. In this presentation, we systematically studied the relationship between Pt nanocubes as nanoscale Pt(100) substrate and different amounts of $Ni(OH)_2$ deposited on Pt(100) surfaces. Pt nanocubes were synthesized under CO gas atmosphere, and then $Ni(OH)_2$ clusters were purposely formed on their surfaces. Well-controlled $Ni(OH)_2$ clusters with different amounts on Pt nanocube surfaces showed volcano-like trend of HER activity in 0.1 M KOH electrolyte.

Oral Presentation : **ELEC.O-6**
Oral Presentation of Young Scholars in Electrochemistry
Room 603+604, THU 09:50
Chair: Sang-Il Choi (Kyungpook National University)

Meniscus configuration of Porous Substrate to Characterize Catalysts for Oxygen Reduction Reaction

Jisu Kim, Hyun Deog Yoo*

Department of Chemistry, Pusan National University, Korea

Oxygen reduction reaction (ORR) is actively utilized for energy storage and conversion, e.g. fuel cells and metal-air batteries. As a four electrons reaction, ORR is kinetically sluggish compared to hydrogen reactions. Therefore, one of the key issues in the catalysis research is developing effective catalysts to decrease the overpotential of ORR. In this regard, it is essential to develop simple and a reliable platform to evaluate catalysts' performance for the discovery of future advanced catalysts. Triple phase boundary (TPB) is the measure of the contact points where O2 (gaseous), electrons (solid), and ions (liquid) meet. Typical rotating disk electrode (RDE) test depends on the dissolved oxygen to characterize ORR activity of a catalyst. However, to build a practical platform to characterize ORR catalysts, TPB should be maximized without vigorous agitation of electrolyte, so that we can simulate the actual operational condition of zinc-air batteries where no artificial agitation is provided. In more detail, a porous carbon paper was slightly contacted to the electrolyte by hooking the center of gravity with a platinum wire, so that the TPB is established among the porous electrode (solid phase), electrolyte (liquid phase), and the air atmosphere (gaseous phase). In addition, the surface tension provided the electric contact for the reliable electrochemical results. The usefulness of this method was demonstrated for Ag and Ag2O catalysts in an alkaline electrolyte, which were successfully applied to operate rechargeable zinc-air batteries. Especially, this meniscus method was especially effective in highly concentrated electrolytes, where RDE test cannot evaluate ORR activity due to the ~3 orders of magnitude lower saturated concentration of dissolved oxygen.

Oral Presentation : **ELEC.O-7**
Oral Presentation of Young Scholars in Electrochemistry
Room 603+604, THU 10:00
Chair: Sang-Il Choi (Kyungpook National University)

Design of organic molecular electrode for aqueous zinc-ion batteries

Moony Na, Hye Ryung Byon*

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

Aqueous zinc-ion batteries (ZIBs) have been revisited for demand on safe and economical rechargeable energy storages. Distinct from typical metal oxide electrodes such as Mn_xO_y used for ZIBs, organic electrodes can provide feasible electrode structure, stable active sites interacting with Zn^{2+} while preventing adverse effect such as the dissolution of Mn^{3+}. Although a few previous studies showed the development of organic ZIB electrodes typically using quinone derivatives, dissolution of organic molecules or remarkable structural change could not be resolved, which caused poor cycling performance. To surmount this challenge, here I present naphthalene diimide (NDI)-based organic electrode for ZIBs. The pi-pi stacking of polycyclic aromatic backbones hindered molecular dissolution and also severe structural change while rendering high electrical conductivity. The carbonyl groups of NDI could store Zn^{2+}during the discharge process. More importantly, H_3O^+ from aqueous electrolyte solution was also observed to insert NDI electrode, which was in fact more attractive to NDI electrode than Zn^{2+} in terms of faster ionic diffusion and less morphological change from monovalent character. The NDI-based organic ZIBs performed stable 1000 cycle with a capacity retention of 97.4% from 105.5 mAh g_{NDI}^{-1} and Coulombic efficiency of 99.1 % I will present details of discharge-recharge mechanism from Zn^{2+} and H_3O^+ co-insertion/desertion for discharge/recharge using various analytical tools.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 10:10

Chair: Sang-Il Choi (Kyungpook National University)

Instability of platinum catalyst in ammonia oxidation reaction

Haesol Kim, Chang Hyuck Choi*

Gwangju Institute of Science and Technology, Korea

Ammonia has received attention as a carbon-free energy carrier, due to its ease of liquefaction and high contents of hydrogen. Ammonia can provide on-site hydrogen production and electricity generation combining with devices, in which platinum shows a promising electrocatalytic activity towards ammonia oxidation reaction (AOR). Many efforts have been made to clarify the poisoning species on the Pt surface, however there is a lack of understanding on the structural/physical deformations of Pt during the AOR which could influence its electrocatalytic stability. In this work, operando dissolution of Pt electrode has been investigated in alkaline ammonia electrolytes using a scanning flow cell system coupled with the inductively coupled plasma mass spectrometer. As similar with the Pt dissolution mechanism in acidic/alkaline electrolytes, Pt ions are leached out under potential-dynamic conditions in ammonia electrolyte, but the dissolution rates (cathodic dissolution in particular) are strongly magnified with increasing ammonia concentrations. UV-VIS spectroscopy study, further confirmed the ligation of ammonia/NOx on Pt ions. Furthermore, the oxidation state and complex structure were investigated by X-ray absorption spectroscopy. These results identify the +4 oxidation state and Pt-N bonding in the dissolved Pt. The ammonia/NOx ligands make Pt ions very stable in alkaline electrolytes, and their electrochemical reduction to metallic Pt require more negative potentials. The results identify that this stabilization of Pt ions leads to the enhanced Pt dissolution and the inhibition of its re-deposition on Pt surface. Stable operando potential windows and operational strategies are further suggested to avoid structural degradation of Pt electrode in ammonia electrolytes.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 603+604, THU 10:20

Chair: Sang-Il Choi (Kyungpook National University)

Co-catalyst onto Fluorinated BiVO4 Photoelectrode for efficient Solar Water Oxidation

Maheswari Arunachalam, Soon Hyung Kang[1,*]

Department of Chemistry, Chonnam National University, Korea
[1]*Department of Chemical Education, Chonnam National University, Korea*

BiVO4 photoanode has been widely investigated due to the narrower bandgap (~ 2.4 eV) that better absorbs visible light, but, disadvantages have also reported in terms of the fast charge recombination process. Herein, we developed the doping of F- ions on BiVO4 films by the fluorination process displayed absorption onset at a wavelength of~ 525 nm, revealing a modest red shift (~14 nm), compared with that of the undoped BiVO4 film. It was notably observed in the pristine BiVO4@Air film improved electronic conductivity through the beneficial electrochemical active sites due to the fluorination induced mixed crystalline-amorphous phase. Furthermore, the deposition of the silver nanowire (Ag NW) as a cocatalyst onto F:BiVO4@Ar film further promotes onset potential (Von) shifts negatively to ～160 mV as well as the increased J values of ~ 2.5 mA/cm2 at 1.23 V vs.RHE, ascribed to the beneficial charge transfer event and high charge transportation rate.

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

General Student Session

Room 602, THU 09:20

Chair: Kiyoung Lee (Kyungpook National University)

Electrochemical Behavior of CO_2 Reduction Reaction on Copper Phosphide Catalyst using in-situ ATR-SEIRAS

Minjun Choi, Jaeyoung Lee*

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

Use of electrochemical method for reduction of carbon dioxide (CO2) convert into valuable organic compounds, is a great solution to solve the problem of CO2 accumulation. The most advantage of electrochemical conversion is to elect reaction to produce a few organic compounds from carbon dioxide depending to types of catalyst. Among many types of catalyst, metal catalysts based on Copper element or alloy metals offers the route to synthesize multi-carbon fuels and chemicals from CO2 (e.g., ethylene, ethanol and n-propanol). In this study, Copper Phosphide was determined by one of the candidate to solve the problem and it was synthesized by oleate method and used as a catalyst in a near Zero-gap CO2 gas-phase electrolytic cell for CO2 reduction reaction at ambient temperature and pressure. By using a hydrophobic gas diffusion layer (GDL), polydimethylsiloxane (PDMS) treated, exhibited the formation of three-phase interphase during the CO2 reduction reaction. The mechanism of the reactions, verified by the onset point of CO adsorption with ATR-SEIRAS, in-situ surface analysis, which is the intermediate of most products by CO2 reduction reaction. GC-MS and UV-Vis equipment was used tool to verify gas/liquid product analysis. Their results show that multi-carbon fuels produced in this reaction.

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

General Student Session

Room 602, THU 09:40

Chair: Kiyoung Lee (Kyungpook National University)

Enhanced Water Splitting of Tungsten Trioxide Photoanode with TiO_2 Overlayer

Cheolwoo Park, Seunghwan Han[1], Tae Kyu Ahn[*], Wooyul Kim[2,*]

Department of Energy Science, Sungkyunkwan University, Korea
[1]*Underwater weapon systems, LIGNEX1, Korea*
[2]*Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea*

Sunlight initiates water oxidation by photogenerated carriers (electr ons and holes) which will follow charge separation processes, charge transfer (injection) and charge recombination during the process. Highly efficient devices for water oxidation have been fabricated through structure modification, deposition of co-catalyst, and surface passivation. Among them, the role of surface passivation hasn't been fully proved yet. Here, we applied uniformed metal oxide passivation layer (prepared by atomic layer deposition, ALD) on tungsten trioxide electrodes to investigate the role of the passivation overlayer by photo induced electrons and holes behaviors. It shows the different photoelectrochemical results depend on metal oxide materials. In particular, transient absorption spectroscopy measurements of WO_3, TiO_2/WO_3 clearly showed that the ultra-fast pathway in the presence of TiO_2 overlayer (ca. ps) under applied bias condition whereas the relatively long-trapped holes portion increased with overlayer, facilitating water photo-oxidation. Detail roles of surface passivation will be presented.

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

General Student Session

Room 602, THU 10:00

Chair: Kiyoung Lee (Kyungpook National University)

Strategies for fast intercalation kinetics of LiCoO2 cathode with high capacity

Fuead Hasan, Jisu Kim, Hyun Deog Yoo*

Department of Chemistry, Pusan National University, Korea

Improving lithium-ion batteries (LIBs)' energy density, rate performance, and cycling stability are pivotal for their utilization in storing renewable energy to address global environmental problems. Therefore, it is highly required to exploit the full capacity and voltage of the cathode materials especially by operating them at higher voltage. Lithium cobalt oxide (LiCoO2, LCO) is a representative cathode in LIBs with excellent electrochemical properties. However, it delivers only half of its theoretical capacity due to the severer side reactions and structural changes at higher cutoff potentials. In this work, we combine two strategies to enhance the intercalation kinetics of LCO cathode: (1) coating lithium ionic conducting lithium phosphate (Li3PO4) and (2) doping various ions as ionic pillars to enable high voltage (4.5 V) and high rate LIBs. Surface engineering by strategy 1 prevents direct contact between liquid electrolytes and lithium cobalt oxide particles, minimizing excessive formation of resistive surface films at high voltage and high temperature. Structural engineering by strategy 2 stabilizes the structure at high voltage, using doped ions (e.g. Mg2+ and Ca2+) as ionic pillars. Combining those strategies can lead to synergetic effect that effectively enhances the energy density, thermal stability, cycling stability, and rate capability. Utilizing the synergetic effect, we have successfully demonstrated excellent rate capability of ~100 mAh/g at 10C-rate (i.e., charge or discharge in 6 min.) and stable cycle performances of ~88% after 100 cycles at 0.5C-rate. Those strategies shed light on the way to more complete and facile exploitation of current cathode materials' energy density.

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

General Student Session

Room 602, THU 10:20

Chair: Kiyoung Lee (Kyungpook National University)

High Performance of Anion Exchange Membrane Water Electrolyzer through pH-Controlled CuCo Oxides Catalyst via Co-Precipitation

Myeong Je Jang, Sungmin Park[1], Sung Mook Choi[2,*]

Advanced Materials Engineering, University of Science & Technology, Korea
[1]*material science & engineering, Pusan National University, Korea*
[2]*Surface Technology Division, Korea Institute of Materials Science, Korea*

An inexpensive, highly efficient and stable electrocatalyst for oxygen evolution reaction is important for the production of pure hydrogen and the commercialization of water electrolysis. In this talk, we reports a highly active nanosized Cu-Co oxide particles for oxygen evolution reaction (OER), through formulating by co-precipitation. We figure that out the catalytic activity of precipitated Cu/Co mixtures is dependent on the ratio of these phases, which can be controlled by the pH of the solution. The oxygen vacancy formed by incorporating Cu into Co^3O^4 and the increase in Co_{3+} due to an increase in pH improved the catalytic activity of oxygen evolution. The nanosized Cu-Co oxide particle exhibits activity with an overpotential of 285 mV at a current density of 10 mA cm^{-2}. Furthermore, the anion exchange membrane water electrolysis cell exhibits the best performance in terms of cell voltage (1.8 V) at 1,300 mA cm^{-2}. This result indicates that Cu-Co oxide can be used as an oxygen evolution reaction catalyst when a full cell is configured.

Oral Presentation : **ENVR.O-5**
General Student Session
Room 602, THU 10:40
Chair: Kiyoung Lee (Kyungpook National University)

Copper cobalt oxide using various precursors for oxygen evolution reaction electrocatalysts by coprecipitation method for AEMWE

Sungmin Park, Myeong Je Jang[1], Sung Mook Choi[2,*]

material science & engineering, Pusan National University, Korea
[1]*Advanced Materials Engineering, University of Science & Technology, Korea*
[2]*Surface Technology Division, Korea Institute of Materials Science, Korea*

Hydrogen energy is considered promising energy to replace fossil fuel because of environmental, infinite energy source and high energy density. In order to produce hydrogen, water electrolysis is suitable method because it can get a high purity of hydrogen without environmental pollution. But high overpotential of oxygen evolution reaction (OER) makes difficult to guarantee of good performance of water electrolysis. To solve these problem, electrocatalyst is necessary for reducing OER overpotential. Nobel metal catalyst such as IrO_2, RuO_2 is well known for ideal oxygen evolution reaction (OER) catalysts, but it has very high cost and scarcity. For this reason, many studies have focused on changing noble metal catalyst to non-noble metal catalyst. Among non-noble metal electrocatalyst, copper cobalt oxide is well known non-noble metal electrocatalyst, because copper cobalt oxide has a good stability and high conductivity. Many methods such as chemical deposition, hydrothermal, electrodeposition and coprecipitation are used to synthesize copper cobalt oxide for electrocatalyst. Especially, coprecipitation is good method for mass production, so it is advantageous for industrial utilization. Moreover, there are various precursors to synthesize by coprecipitation, however It is not known which precursors represent the best OER performance. In this study, we suggest the effect of morphology and activity control in precursor to copper cobalt oxide structures. Synthesized copper cobalt oxide OER catalysts is recorded the overpotential of 364 mV at 10 mA/cm^2 and low Tafel slope of 73.76 mV/dec in 1 M KOH. In addition, the synthesized catalyst is applied to the anode of the actual AEMWE cell through an electrode process.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

Living Cascade Polymerization via Tandem Olefin Metathesis /Metallotropic 1,3-Shift Reactions for the Synthesis of Conjugated Polyenynes

Cheol Kang, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

Since the first discovery in 1969, polyenynes received much attention due to their intriguing optoelectronic properties that made them useful materials for molecular sensors. Although there have been extensive studies for the synthesis of various polyenynes, only a handful of polyenyne motifs were reported to date. Furthermore, most of the synthetic routes to polyenynes relied on topochemical synthesis in solid state, limiting their versatility in applications due to poor solubility. Even though the syntheses of soluble polyenynes were possible by step-growth mechanism, preparation of conjugated polyenynes with high molecular weights in a controlled manner remained elusive.

Very recently, we developed a new cascade polymerization method by combining two different organic reactions; olefin metathesis and metallotropic 1,3-shift. By rationally designing stable multialkyne monomers, a series of metathesis and metallotropy reactions proceeded by Grubbs catalyst in a sequence-specific manner to afford conjugated polymers containing unique polyenyne motifs in their backbone. For example, tetradeca-1,6,8,13-tetrayne moieties underwent a cascade transformation of ring-closing/metallotropic 1,3-shift/ring-closing reactions in a sequence-specific manner to efficiently generate a conjugated polyenyne backbone with a Z-E-Z alkene sequence and one triple bond. In addition to this tetrayne monomers, other two classes of monomers, pentaynes and hexaynes, underwent remarkably complex cascade reactions (up to 5 independent transformations) at high levels of selectivity to afford unprecedented conjugated polyenyne structures. This new polymerization, which we call cascade metathesis and metallotropy (M&M) polymerization, is the first example of making polyenynes by chain-growth mechanism, which enabled the precise control over molecular weights with narrow dispersities. Furthermore, living M&M polymerization realized the synthesis of block copolymers consisting of fully conjugated polyenyne backbones which highlights the uniqueness and versatility of M&M polymerization.

Oral Presentation : **KCS.O-0**
Oral Presentation for 2019 DOW Korea Award
, SUN :

Unravelling Excited Singlet State Aromaticity via Vibrational Analysis

Juwon Oh, Young Mo Sung, Hirotaka Mori[1], Seongchul Park[2], Kjell Jorner[3], Henrik Ottosson[3], Manho Lim[2], Atsuhiro Osuka[1,*], Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea
[1]*Department of Chemistry, Graduate School of Science, Japan*
[2]*Department of Chemistry, Pusan National University, Korea*
[3]*Department of Chemistry, Uppsala University, Sweden*

Aromaticity, the special energetic stability derived from cyclic [4n+2]π-conjugated electronic structures, has been the topic of intense interest in chemistry because it plays a critical role in rationalizing molecular stability, reactivity, and physical/chemical properties. Recently, the pioneering work by Colin Baird on aromaticity reversal, postulating that aromatic (antiaromatic) character in the ground state reverses to antiaromatic (aromatic) character in the lowest excited triplet state, has attracted much scientific attention. The completely reversed aromaticity in the excited state provides direct insight into understanding the photo-physical/chemical properties of photo-active materials. In turn, the application of aromatic molecules to photo-active materials has led to numerous studies revealing this aromaticity reversal. However, most studies on excited state aromaticity have been based on the theoretical point of view. The experimental evaluation of aromaticity in the excited state is still challenging and strenuous because the assessment of (anti)aromaticity with conventional magnetic, energetic, and geometric indices is difficult in the excited state, which practically restricts the extension and application of the concept of excited state aromaticity.Time-resolved optical spectroscopies can provide a new and alternative avenue to experimentally evaluate excited state aromaticity while observing changes in the molecular features in the excited states. Time-resolved optical spectroscopies take advantage of ultrafast laser pulses for achieving high time resolution, which are suitable for monitoring ultrafast changes in the excited state of molecular systems. This will provide valuable information for understanding the aromaticity reversal.Here, as a new and unconventional approach, time-resolved IR (TRIR) spectroscopy on aromatic/antiaromatic hexaphyrin congeners shed light on the excited singlet state aromaticity. Expanded porphyrins exhibit perfect aromatic and antiaromatic congener pairs, having the same molecular framework but with different numbers of π-electrons, which facilitates the study on the pure effect of aromaticity by comparative analyses. The contrasting spectral features between the FT-IR and TRIR spectra reveal the aromaticity-driven structural changes, strongly corroborating aromaticity reversal in the excited singlet states. Our new paradigm for the excited state aromaticity, the correlation of IR spectral features with aromaticity reversal, provides another fundamental key to understanding the role of (anti)aromaticity in the stability, dynamics and reactivity in the excited singlet state of π-conjugated molecular systems.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

A Nonheme Manganese(III)-Iodosylarene Complex: Synthesis, Characterization and Electrophilic Reaction

Donghyun Jeong, Takehiro Ohta[1], Jaeheung Cho[*]

Emerging Materials Science, DGIST, Korea

[1]*Picobiology Institute, Graduate School of Life Science, University of Hyogo, Japan*

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

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

The Chemical Fluctuation Theorem governing gene expression

Seong-jun Park, Sanggeun Song[1], Gil-Suk Yang[2], Philip M. Kim[3], Sangwoon Yoon[4,*], Ji-Hyun Kim[2,*], Jaeyoung Sung[1,*]

Creative Research Initiative Center for Chemical Dynamics in Living Cells, Chung-Ang University / National Institute of Innovative Functional Imaging, Chung-Ang University, Korea

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[3]*Terrence Donnelly Center for Cellular and Biomolecular Research, Department of Molecular Genetics and Department of Computer Science, University of Toronto, Toronto M5S 3E1 ON, Canada*

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

Gene expression is a complex stochastic process composed of numerous enzymatic reactions with rates coupled to hidden cell-state variables. Despite advances in single-cell technologies, the lack of a theory accurately describing the gene expression process has restricted a robust, quantitative understanding of gene expression variability among cells. Here we present the Chemical Fluctuation Theorem (CFT), providing an accurate relationship between the environment-coupled chemical dynamics of gene expression and gene expression variability. Combined with a general, accurate model of environment-coupled transcription processes, the CFT provides a unified explanation of mRNA variability for various experimental systems. From this analysis, we construct a quantitative model of transcription dynamics enabling analytic predictions for the dependence of mRNA noise on the mRNA lifetime distribution, confirmed against stochastic simulation. This work suggests promising new directions for quantitative investigation into cellular control over biological functions by making complex dynamics of intracellular reactions accessible to rigorous mathematical deductions.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

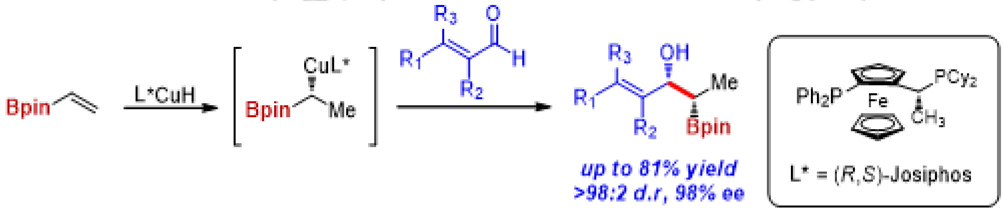
, SUN :

Copper-Catalyzed Tandem Hydrocupration and Diastereo- and Enantioselective Borylalkyl Addition to Aldehydes

Won Jun Jang, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

We report the copper-catalyzed stereoselective addition of in situ generated chiral boron-α-alkyl intermediates to various aldehydes including α,β-unsaturated aldehydes under mild conditions. This tandem and multicomponent method facilitated the synthesis of enantiomerically enriched 1,2-hydroxyboronates bearing contiguous stereocenters in good yield with high diastereo- and enantioselectivity up to a ratio greater than 98:2. In particular, α,β-unsaturated aldehydes were successfully used as electrophiles in Cu−H catalysis through 1,2-addition without significant reduction. The resulting 1,2-hydroxyboronates were used in various transformations.



Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

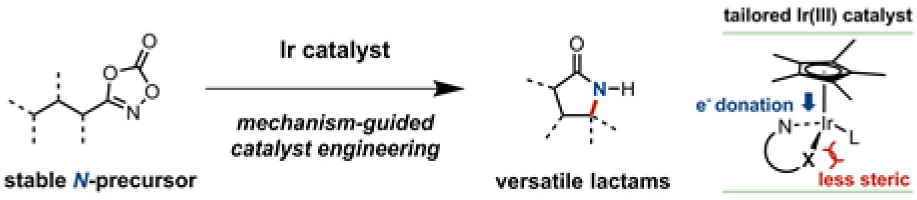
, SUN :

Selective formation of γ-lactams via C–H amidation enabled by tailored iridium catalysts

Seung Youn Hong, Yoonsu Park, Yeongyu Hwang, Yeong Bum Kim, Mu-Hyun Baik*, Sukbok Chang*

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

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



Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

π-Conjugated Polymers Incorporating a Novel Planar Quinoid Building Block with Extended Delocalization and High Charge Carrier Mobility

Yunseul Kim, Hansu Hwang, Nam-Koo Kim, Kyoungtae Hwang, Jong-Jin Park, Ga-In Shin, Dong-Yu Kim[*]

School of Materials Science and Engineering (SMSE), Gwangju Insititute of Science and Technology (GIST), Korea

Conjugated polymers have been extensively studied as organic semiconductors and investigated for various applications such as flexible displays and printed electronics due to their mechanical flexibility and solution processability. In particular, molecular design, synthesis, and structure-property relationship of π-conjugated polymers have been intensively researched. A quinoid structure is a molecular conformation in which aromatic rings are connected by double bonds. Their high molecular planarity arisen from double bond linkage induces a favorable intramolecular π-electron delocalization and an efficient intermolecular overlap of π-orbitals, leading to improving charge transport. Moreover, they have unique features such as low electronic band-gap and amphoteric redox properties. Here, we present two conjugated polymers, PQuT-T and PQuT-BT, incorporating quinoidal thiophene by substituting isatin termini. By combining 1D-, 2D-COSY, and NOESY NMR analyses, the isomeric form of the major quinoidal moiety is clearly identified as the asymmetric *Z, E*-configuration. These quinoidal moiety contributed greatly not only to narrow band-gap but also to achieve high mobility in organic field-effect transistors. Charge transport properties of quinoidal polymers are enhanced by chain alignment via simple solution processing technique using centrifugal force, with PQuT-BT exhibiting a high hole mobility of 8.09 cm^2/Vs.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

New Approach for Large-Area Thermoelectric Junctions with a Liquid Eutectic Gallium−Indium Electrode

Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Studies of thermopower in molecular junctions permit access to the atomic-detailed energy topography across junctions and how thermopower is associated with chemical structure of the active molecular components inside junctions. This presentation describes a liquid metal-based thermoelectric junction technique and structure-thermopower relationships established with the technique. Cone-shaped liquid Ga-In alloy (EGaIn) microelectrode allows us to achieve high yields of working junctions and thus statistically sufficient thermoelectric data sets. We estimated thermopowers of EGaIn and the Ga_2O_3 layer on the EGaIn conical tip and successfully validated our platform with widely studied molecules, oligophenylene thiolates.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

Single-Crystal Poly[4-(4,4-dihexadecyl-4H-cyclopenta[1,2-b:5,4-b′]dithiophen-2-yl)-alt-[1,2,5]thiadiazolo[3,4-c]pyridine] Nanowireswith Ultrahigh Mobility

Yoonkyoung Park, Jin Won Jung, Hungu Kang, Jhumur Seth, Youngjong Kang, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

We fabricated single-crystal poly[4-(4,4-dihexadecyl-4H-cyclopenta[1,2-b:5,4-b′]-dithiophen-2-yl)-alt-[1,2,5]thiadiazolo-[3,4-c]pyridine] (PCDTPT) nanowires with ultrahigh mobility using a liquid-bridge-mediated nanotransfer molding method. The structural analysis of the singlecrystal PCDTPT nanowires reveals that PCDTPT crystals have a triclinic structure, and the nanowires grow parallel to PCDTPT backbone chains, which provide important insights into its intrinsic charge transport. The single-crystal PCDTPT nanowire exhibits a superior charge carrier mobility of 72.94 ± 18.02 cm^2 V^{-1} s^{-1} (maximum mobility up to 92.64 cm^2 V^{-1} s^{-1}), which is a record high value among conjugated polymers to date. In the single-crystal PCDTPT nanowire, the backbone chains in the linear structure along the nanowire growth axis lead to strong backbone delocalization, resulting in highlyconductive polymer backbones and a drastic increase in charge carrier mobility. In addition, the single-crystal PCDTPT nanowire shows good environmental stability under air conditions compared to small-molecule organic semiconductors.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

Direct Synthesis of a Covalent Triazine-Based Framework from Aromatic Amides

Soo-Young Yu, Javeed Mahmood, Hyuk-Jun Noh, Jeong-Min Seo, Sun-Min Jung, Sun-Hee Shin, Yoon-Kwang Im, In-Yup Jeon[1], Jong-Beom Baek[*]

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemical Engineering, Wonkwang University, Korea*

There have been extensive efforts to synthesize crystalline covalent triazine-based frameworks (CTFs) for practical applications and to realize their potential. The phosphorus pentoxide (P_2O_5)-catalyzed direct condensation of aromatic amide instead of aromatic nitrile to form triazine rings. P_2O_5-catalyzed condensation was applied on terephthalamide to construct a covalent triazine-based framework (*p*CTF-1). This approach yielded highly crystalline *p*CTF-1 with high specific surface area (2034.1 $m^2 g^{-1}$). At low pressure, the *p*CTF-1 showed high CO_2 (21.9 wt% at 273 K) and H_2 (1.75 wt% at 77 K) uptake capacities. The direct formation of a triazine-based COF was also confirmed by model reactions, with the P_2O_5-catalyzed condensation reaction of both benzamide and benzonitrile to form 1,3,5-triphenyl-2,4,6-triazine in high yield.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

The effect of Initial Condition in Oxidized Cu for Stable and Selective Ethylene Production from Electrochemical CO_2 Reduction

Si Young Lee, Yun Jeong Hwang[1,*]

Division of Energy and Environmental Technology, KIST School, Korea University of Science and Technology / Clean Energy Research Center, Korea Institute of Science and Technology, Korea

[1]*Division of Energy and Environmental Technology, KIST School, Korea University of Science and Technology / Clean Energy Research Center, Korea Institute of Science and Technology / College of Engineering, Yonsei University, Korea*

Recently, in electrochemical CO_2 reduction studies, copper catalysts have been noted as major studies because they could form C-C bonds. To promote the formation of this C-C bond, researchers changed the shape of the copper catalyst surface to induce local pH changes, or to introduce copper oxide as a catalyst. However, in copper oxide-based catalysts not only complexly synthesizes the catalyst, it is not clear why the oxide catalyst shows better C-C coupling performance. Therefore, in this study, a simple anodization method was introduced to synthesize the catalyst in the $Cu(OH)_2$ state. This catalyst was distinguished from the Cu_2O or CuO present in the traditional native oxide layer, and showed a 40% ethylene selectivity, which was twice as good as copper foil, stable for 40 hours. On the other hand, uniquely selectivity of CH_4 increased slightly over time in the long-term bulk electrolysis. This means that the C1/C2 generation ratio changes with changes in surface conditions of $Cu(OH)_2$ catalyst. Therefore, we introduced pre-treatment process, which is high negative potential reduction and low negative potential reduction to adjust the $Cu^{2+}/Cu^{+}/Cu^{0}$ ratio of the surface. At this time we observed that while ethylene production was stable for a long time for samples with a high ratio of Cu^{2+}, samples with missing Cu^{2+} decreased ethylene production and increased methane production rapidly within hours. Not only could the cause of C-C bond formation of copper catalyst be identified through this study, it could present a new strategy to maintain stability in oxide-derived copper catalyst in the future.

Oral Presentation : **KCS.O-0**

Oral Presentation for 2019 DOW Korea Award

, SUN :

Structural features and their functions in surfactant-armoured methylammonium lead iodide perovskites for highly efficient and stable solar cells.

Minsu Jung, Tae Joo Shin[1], Jangwon Seo[2], Gwisu Kim, Sang Il Seok*

School of Energy and Chemical Engineering, UNIST, Korea
[1]*UNIST Central Research Facilities, UNIST, Korea*
[2]*Division of Advanced Materials, Korea Research Institute of Chemical Technology, Korea*

Methylammonium lead iodide perovskites have limited practical applications due to a lack of stability under operating conditions. Environmental stability under heating has not yet been achieved, although recent studies modifying perovskites with long organic cations have reported the progress of stabilisation under humid conditions. In this work, we report the structural evolution of long alkylammonium-modified $MAPbI_3$ and its functions for highly efficient and stable solar cells. As an encapsulating agent, octylammonium (OA) cation produced individual $MAPbI_3$ grains in full armour without the formation of layered structures in contrast to butylammonium (BA) and phenethylammonium (PEA) cations. Our OA-armoured $MAPbI_3$ achieved a stabilised power conversion efficiency of 20.1% without a deterioration of charge transport properties due to highly preferential orientation suppressing non-radiative recombination. The structural features also led to a much improved thermal stability at 85 ˚C in ambient atmosphere retaining 80% of the initial efficiency after 760 h without any encapsulation, as well as water tolerance. This work addresses widespread concerns associated with the photovoltaic efficiency and stability of $MAPbI_3$ by exploring the inter-relationship between structural features and their functions in surfactant-modified perovskites.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and ring-opening polymerization of alpha-amino acid N-carboxyanhydrides

Ji hoon Lee, **Kyung-sun Son***

Department of Chemistry, Chungnam National University, Korea

The synthesis of polypeptides using α-amino acids plays an important role in the field of biomaterials. The unique features of these functional polypeptides including their chemical diversity of side chain enable broad applications in the field of protein/peptide mimicking, drug/gene delivery, tissue engineering, and other practical applications of biomaterials. Synthetic polypeptides were prepared by ring opening polymerization of α-amino acid N-carboxyanhydrides (NCAs) via a convenient procedure using lithium hexamethyldisilazide (LiHMDS) as an initiator in an open vessel with a minimum use of glove box or Schlenk line. The living NCA polymerization method allowed the preparation of synthetic polypeptide libraries in an efficient manner.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Relationship between the light sources and performance of organic photocatalysts in organo-catalyzed atom transfer radical polymerization

Chung Soo Kim, Jisu Back[1], Eunsung Lee[1,*], Kyung-sun Son[2,*]

Chungnam National University, Korea

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

[2]*Department of Chemistry, Chungnam National University, Korea*

We studied the relationship between light sources and performance of organic photocatalysts (PCs) for metal-free atom transfer radical polymerization process (ATRP). The initiation efficiency and dispersity of polymers produced by organocatalyzed ATRP were highly affected by the light sources such as white LEDs, compact fluorescent lamp (CFL), and sunlight. The effects of the light sources on the PC's performance were systematically investigated.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Alternating ring-opening copolymerization using a sterically demanding chromium complex

Ho Kyun Ryu, Dae Young Bae[1], Eunsung Lee[1], Kyung-sun Son[2,*]

Chungnam National University, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*
[2]*Department of Chemistry, Chungnam National University, Korea*

Ring-opening copolymerization (ROCOP) of epoxides with anhydrides was performed using a chromium complex containing sterically-demanding amino triphenolate ligand and a series of co-catalysts. The polymerization results employing the chromium complex was affected by the type and the amount of co-catalyst, reaction time, and the ratio of monomers. After optimization of reaction conditions, the chromium complex successfully produced well-define polyesters with high molecular weights, high glass-transition temperatures, and low polydispersity.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Zr(IV)-Mediated, Versatile Heparin Coating on Solid Surfaces for Antiplatelet Application

Yeonwoo Jeong, Sung Min Kang*

Department of Chemistry, Chungbuk National University, Korea

Control over platelet adhesion on artificial surfaces has been of great interest because non-specific adhesion of platelet on solid surfaces can cause biomedical devices to malfunction. To avoid these problems, heparin coating has been extensively used. However, previous approaches for heparin coating showed several drawbacks: complicated and time-consuming steps are required. Herein, we developed a facile heparin coating method. Solid surfaces were pretreated with tannic acid/Zr(IV) complexes. Heparin was then deposited on the surface through a spin-coating process and fixed by Zr(IV) mediated crosslinking reaction. Using this approach, TA/Zr(IV)/heparin coatings that are highly resistant to human platelet adhesion were successfully formed on various substrates.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Role of fluorescent Waste Tea Residue -Carbon Dots (WTR-CDs) hybrid thin films on blocking the Ultra-violet radiations as direct application

Govind Kolekar, Daewon Sohn[1,*]

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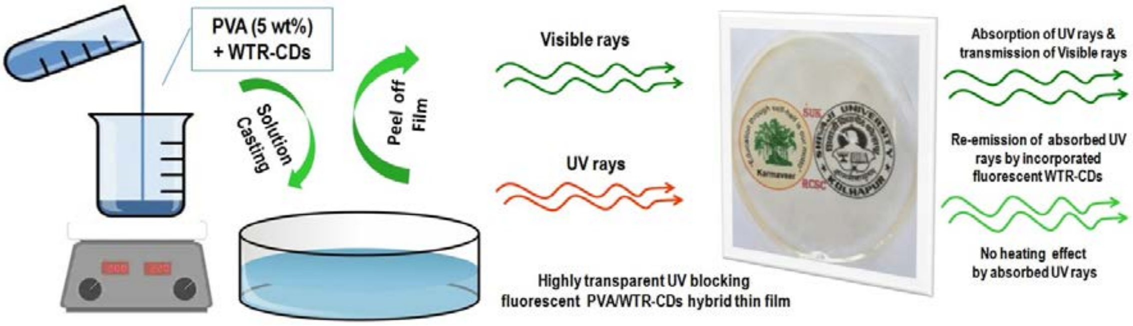
Everyone is exposed to UV radiation from the sun and increasing number of people are exposed to artificial sources used in industry. Emissions from the sun includes visible light, heat and UV radiation. UV radiation is beneficial for the production of vitamin D which helps the body absorb calcium and phosphorus from the food and bone development. However, in environmental abundance, UV is the most risk factor for skin cancer and many other environmentally influenced skin disorders. Overexposure to UV radiation can cause cancer which is common in the united states. The two most common types of skin cancer are basal cell cancer and squamous cell cancer. Typically, they form on the head, face, neck, hands and arms because these body parts are the most exposed to UV radiation. Most cases of melanoma, the deadliest kind of skin cancer are caused by exposure to UV radiation. Therefore, the world health organization (WHO) recommends 5 to 15 minutes of sun exposure 2 to 3 times in a week. Herein we have fabricated the waste tea residue carbon dots (WTR-CDs) as a hybrid thin films used for UV blocking agents. The incorporated fluorescent WTR-CDs impart fluorescence to the whole film and films are capable to not only block the UV region but also reemit absorbed UV light into the visible region. We achieved the maximum percent of UV blocking by Polyvinylalcohol (PVA) -WTR-CDs-5 film by controlling the transparency and thickness. By the successive addition of UV blocking agent, there was no extreme changes were observed in the intrinsic mechanical as well as tensile properties of PVA films. The multidynamic properties of prepared PVA/WTR-CDs hybrid films can prove its applicability for pharmaceutical storage, packaging, wrapping and coating in diverse fields.


PVA (5 wt%)
+ WTR-CDs
Solution Casting
Peel off Film
Visible rays
UV rays
Highly transparent UV blocking
fluorescent PVA/WTR-CDs hybrid thin film
Absorption of UV rays &
transmission of Visible rays
Re-emission of absorbed UV
rays by incorporated
fluorescent WTR-CDs
No heating effect
by absorbed UV rays

Poster Presentation : **POLY.P-6**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Injectable, biocompatible conjugated catechol chitosan hydro-gels with ion inducement and ethylenediamine tetra-acetic acid treatment

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Chitosan (CS) is a natural polycationic polysaccharide and pH-sensitive polymer with incomplete deacetylation from claiming chitin. It is also a guaranteeing material in terms of pharmaceutical, chemical, and sustenance industry due to its exceptional structure including reactive –OH and –NH2 groups. In this study, catechol-modified chitosan (CCS) for an eminent level for substitution was synthesized and propelled by marine mussel cuticles in place on research those intricate connections between Fe3+ and catechol under acidic conditions. The ratios of catechol, chitosan, and other reagents decide the structure of the hydrogel. The gel formation is then well-maintained by dual cross-linking through electrostatic interactions between CCS and oxidative ions such as Fe3+ and IO4- through covalent catechol-coupling-based coordinate bonds. The hydrogels showed enhanced cohesiveness and shock-absorbing properties at lower pH and ethylenediaminetetraacetic acid (EDTA) treatment due to coordinate bonds inspired by mussel byssal threads. Thus, the gelation time, rheological properties, UV-vis and 1H- Nuclear Magnetic Resonance spectroscopy, and the morphologic aspects were elucidated to describe those cross-linking components and the physical properties of the chitosan backbones and hydrogel frame-works.

Poster Presentation : **POLY.P-7**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Dynamic Imine Polymeric Micelles for Efficient Drug Delivery

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For an efficient drug delivery system (DDS), releasing the drug at a desired site is essential as well as insuring the stability of the drug under physiological conditions. Due to the acidic pH conditions of tumor cell, dynamic covalent imine bond can be exploited as a key chemistry for a stimuli-responsive DDS. In this study, we designed and synthesized the novel diblock copolyethers composed of functional epoxide monomers of ethoxy ethyl glycidyl ether (EEGE) and a novel azido-hexyl glycidyl ether (AHGE) via sequential anionic ring-opening polymerization (AROP) using organic superbase, t-BuP_4. After the successful polymerization, the corresponding acetal group in P(EEGE) was deprotected to hydroxyl group and azide group in P(AHGE) was modified to amine through Staudinger reduction. A series of the AB-type diblock copolymers of P(EEGE-*b*-AHGE) were carefully characterized by ^{1}H NMR, GPC, and FT-IR. The prepared double hydrophilic block copolymer of P(EEGE-*b*-AHGE) was conjugated with a potential anticancer agent, cinnamaldehyde, through the imine linkage to afford the amphiphilic block copolymer to self-assemble into a polymeric micelles in physiological conditions. The selective release under acidic pH conditions led to a cleavage of the imine bond and release of cinnamaldehyde with a concomitant disassembly of polymeric micelles. We anticipate this dynamic imine linkage will afford a conjugation of various functional therapeutic agents for a smart DDS.

Poster Presentation : **POLY.P-8**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Preparation and Characterization of a Novel Polyimide/Surface Modified $BaTiO_3$ Nanocomposite for Solution Processable High k Dielectric

Kyeongmin Kim, Taek Ahn*

Department of Chemistry, Kyungsung University, Korea

The development of high performance flexible electronics requires dielectrics possessing a high dielectric constant and enhanced mechanical stability. In this study, we report on a novel polymer nanocomposite dielectric based on 3-glycidoxypropyltrimethoxysilane (GPTES) functionalized barium titanate ($BaTiO_3$) nanoparticle as a dopant in crosslinkable polyimide. Firstly, the hydroxyl group containing polyimide (DOCDA-6FHAB) polymer was synthesized through a simple one step condensation polymerization using the monomers, 5-(2,5-dioxytetrahydrofuryl)3-methly-3- cyclohexene-1-2-dicarboxylic anhydride (DOCDA) and 2,2-bis(3-amino-4-hydroxyphenyl)hexafluoropropane (6FHAB). And then, we introduced the barium titanate ($BaTiO_3$) nanoparticle to make a high dielectric constant polyimide nanocomposite dielectric. To avoid the large leakage current and low breakdown strength, control over the particle-particle interaction and particle-polymer interface is essential. Thus, approaches to modify nanoparticles via robust chemical bonds are highly desirable. Therefore, the surface of barium titanate was modified by 3-glycidoxypropyltrimethoxysilane (GPTES) to increase the interfacial adhesion between polyimide and nanoparticle. In addition, we used crosslinked poly(4-vinylphenol) (PVP) as capping layer on polyimide nanocomposite layer to further improve leakage current and surface roughness. Polyimide nanocomposite was systematically characterized such as chemical structures, surface roughness, surface energy, and capacitance, etc. Polyimide nanocomposite bilayer film showed high dielectric constant (5.58) and low leakage current density (10^{-7} A/cm^2) in metal-insulator-metal devices. Detailed synthetic routes of polyimide and nanocomposite film fabrication condition will be presented.

Poster Presentation : **POLY.P-9**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Thin Film Properties of a Novel Polyimide/Surface Modified TiO_2 Nanocomposite Layer for Solution Processable High k Dielectric

Kyeongmin Kim, Taek Ahn*

Department of Chemistry, Kyungsung University, Korea

For high performance organic thin film transistors (OTFTs), OTFT require dielectrics having a high dielectric constant and enhanced mechanical stability. In this study, we report on a novel polymer nanocomposite dielectric based on a (3-aminopropyl)triethoxysilane (APTES) functionalized titanium dioxide (TiO_2) nanoparticle as a dopant in crosslinkable polyimide (PI). Firstly, the hydroxyl group containing polyimide (DOCDA-6FHAB) polymer was synthesized through a simple one step condensation polymerization using the monomers, 5-(2,5-dioxytetrahydrofuryl)3-methly-3- cyclohexene-1-2-dicarboxylic anhydride (DOCDA) and 2,2-bis(3-amino-4-hydroxyphenyl)hexafluoropropane (6FHAB). And then, we introduced the titanium dioxide (TiO_2) nanoparticle to make a high dielectric constant polyimide nanocomposite dielectric. To avoid the large leakage current and low breakdown strength, control over the particle-particle interaction and particle-polymer interface is essential. Thus, approaches to modify nanoparticles via robust chemical bonds are highly desirable. Therefore, the surface of titanium dioxide (TiO_2) was modified by (3-aminopropyl)triethoxysilane (APTES) to increase the interfacial adhesion between polyimide and nanoparticle. In addition, we used crosslinked DOCDA-6FHAB as capping layer on polyimide nanocomposite layer to further improve leakage current and surface roughness. Polyimide nanocomposite was systematically characterized such as chemical structures, surface roughness, surface energy, and capacitance, etc. Polyimide nanocomposite bilayer film showed high dielectric constant (5.51) and low leakage current density (10^{-7} A/cm^2) in metal-insulator-metal (MIM) devices. Detailed synthetic routes of polyimide and nanocomposite film fabrication condition will be presented.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Syntheses and Characterization of Donor-acceptor Polymers Based on Polyphenazine with BDT Derivatives for Solar Cells

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[2]*Engineering Chemistry, Pukyong National University, Korea*

Research on organic solar cells is being actively conducted. Organic solar cells have many merit than inorganic solar cell, but are slightly difficult to commercialize because of their low conversion efficiency. Effect factor of conversion efficeinecy in organic solar cells is HOMO value, band gap, charge career mobility and so on. The lower the HOMO, the narrower the band gap, the better the charge mobility, the better the efficiency can be. DFPz can have low HOMO because it has two fluorine atoms and two nitrogen atoms that have strong withdrawing effect, and polymerization with BDTT so it can have small bandgap. Phenazine has extended benzene ring than quinoxaline units so it attribute good charge mobility to DFPZ's smoothness and high efficiency organic solar cell can be made based on this. One of donor material is PBDTT-DoDFPZ and other PBDTT-DHDFPz and acceptor unit used PCBM. The result of PCE in PBDTT-DoDFPZ is 2.76% which is higher than PBDTT-DT-DoDFP's power conversion efficiency of 2.73%.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Properties of Alternating Copolymers Based on Fluorinated Phenazine

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[1]*Department of Polymer?Engineering, Pukyong National University, Korea*
[2]*Engineering Chemistry, Pukyong National University, Korea*

Recently, there are many research of renewable energy. PSC(polymer solar cell) having remarkable advantage including flexible, large area application and facile tuning by substituting functional group is one of them. In the active layer material for high efficiency, to obtain proper HOMO(highest occupied molecular orbital) and LUMO(lowest unoccupied molecular orbital) energy level and high charge carrier mobility of polymers, D-A alternating structure was introduced. Benzodithiophene was used as donor unit, And diflourinated phenazine(DFPz) was used as accepter unit. Phenazine unit can be fine materials for the PSC because it has C=N bond (strong electronegativity) and extended π conjugated structure for high hole mobility. To check the effect of alkyl side chain, either linear alkyl chain or bulky alkyl chain was introduced to the resulting copolymers. As a result, PBDT-DT_DoDFPz was red-shifted than PBDT-DT-DHDFPz. This can be attributed to that the polymer with linear alkyl chain was better packed in film than polymer with a branched alkyl side chain. Finally, the polymer with linear alkyl chain (PBDT-DT-DoFPz) achieved 3.41% of PCE.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Water absorption of random poly(styrene-co-itaconate) (PSITA) ionomers and PSITA / PEG blends

Joon-Seop Kim*, Yoon Gwan Jeong[1]

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[1]*Department of Polymer chemistry Engineering, Chosun University, Korea*

In this study, we compared the water absorption of random poly(styrene-co-itaconate) (PSITA) ionomers and PSITA / PEG blends. The contents of PEG (average molecular weight = 4000) of the PSITA / PEG blend were 10 and 20 wt%. In this experiment, the acid groups of the copolymers were completely neutralized with NaOH and LiOH to make PSITA ionomers. The results showed that the ionomers blended with PEG absorbed more water than the pure PSITA ionomers. On the other hand, when comparing the water absorption of Li-ionomer blends and Na-ionomer blends, water absorption was increased up to 2 wt% in case of Li-ionomer blends, but up to 10 wt% in case of Na-ionomer blends. It was found that the water absorption of the blends was more than pure ionomers. It was also observed that the water absorption was affected by the blended PEG content and the type of cations of the ionomers.

Poster Presentation : **POLY.P-13**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of 1,1-Diisopropyl(or dihexyl)-2,5-ethynyl-3,4-diphenyl-siloles and their Glaser Oxidative Coupling Polymerization Reactions

Jong Wook Lim, Young Tae Park[1,*]

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2,5-Dibromo-1,1-diisopropyl(or dihexyl)-3,4-diphenyl-siloles were prepared by reactions of diisopropyl(or dihexyl)-bis(phenylethynyl)silanes with lithium naphthalenide, $ZnCl_2$, and *N*-bromosuccinimide (NBS). Palladium chloride, copper iodide, and triphenylphosphine as co-catalyst were used to replace two bromine groups of the prepared siloles with trimethylsilylacetylene (TMSA) under the reaction condition of diisopropylamine as solvent, in which were produced 1,1-diisopropyl(or dihexyl)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles. Then, detrimethylsilylation reactions were carried out to yield 1,1-diisopropyl(or dihexyl)-2,5-bis(ethynyl)-3,4-diphenyl-siloles using potassium carbonate under the methanol as solvent. The crude products were refined by recrystallization or column chromatography in the solvent of hexane. The product materials were characterized by ^{1}H, ^{13}C, and ^{29}Si NMR. We also studied the photoelectronic properties of the materials by UV-vis absorption, excitation and fluorescence emission spectroscopic methods. We will also try Glaser oxidative coupling polymerization reactions of 1,1-diisopropyl(or dihexyl)-2,5-bis(ethynyl)-3,4-diphenyl-siloles in the presence of a catalytic amount of copper(I)chloride and pyridine with bubbling oxygen gas through reaction mixture to yield poly(1,1-diisopropyl(or dihexyl)-2,5-bis(ethynylene-3,4-diphenyl-silole)s. Acknowledgment. This work was supported by the Basic Science Research Program through the Nationaril Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2017R1D1A3B03028014).

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Co-oligomerization Reactions of 2,5-Dibromo-1,1-diisopropyl (or dihexyl)-3,4-diphenylsiloles with 4,4'-(Hexafluoroisopropylidene)diphenol (or Bisphenol A or 4,4'-Biphenol) and their Characterizations

Jong Wook Lim, Young Tae Park[1,*]

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

2,5-Dibromo-1,1-diisopropyl(or dihexyl)-3,4-diphenyl-siloles were prepared by reactions of diisopropyl (or dihexyl)-bis(phenylethynyl)silanes with lithium naphthalenide, anhydrous $ZnCl_2$, and *N*-bromosuccinimide (NBS), respectively. Co-oligomerizations of the prepared silole derivatives with 4,4'-(hexafluoroiso-propylidene)diphenol, bisphenol A, and 4,4'-biphenol as co-monomers were carried out by the nucleophilic substitution reactions of two bromine groups in the presence of potassium carbonate under the co-solvent of *N*-methyl-2-pyrrolidinone (NMP) and toluene with Dean-Stark trap. The crude product was purified by extraction using the solvents of dichloromethane and washed with deionized water. The product materials were characterized by ^{1}H, ^{13}C, and ^{29}Si NMR as well as GPC. We also studied the photoelectronic properties by UV-vis absorption, excitation, and fluorescence emission spectroscopic methods, in particular, along with electrochemical properties. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2017R1D1A3B03028014).

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Investigation of dithienosilole-co-5-fluoro-2,1,3-benzothiadiazole-containing polymeric regioisomers for organic field-effect transistors

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[2]*chemical engineering/advancer materials, Dongseo University, Korea*

Three polymeric regioisomers polymers (P1, P2, and P3) containing dithienosilole (DTS) and 5-fluoro-2,1,3-benzothiadiazole moieties are synthesized and characterized. Even if all the polymers exhibit similar energy levels, they show different crystallinity, molecular orientation, and charge-carrier transporting characteristics. A hole mobility (0.021 cm2 V-1s-1) is demonstrated for organic field-effect transistor (OFET)-based on P3 with the geometrical same direction of F atoms, which is much higher than the regiorandom (P1) and regioregular (P2) oriented isomers. Our study uncovers that the specific regio-orientation of the asymmetric units rather than the regioregularity in the backbone plays a crucial role in determining the polymer nature, bulk morphology, and OFET performance.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Interfacial behavior of amphiphilic heteroarm core cross-linked star polymers

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Core cross-linked star (CCS) polymers possess polymer arms radiating from a cross-linked core. Amphiphilic heteroarm CCS polymer containing both hydrophilic and hydrophobic arms is expected to stabilize oil/water interface more effectively than the linear analogue if the two arms are intramolecularly segregated. We will discuss feasible synthesis of such an amphiphilic heteroarm CCS polymer based on "in-out" approach, and report their self-assembly behavior and interfacial properties.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Supramolecular chirality from internal and external origins

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Supramolecular chirality typically originates from the chiral information of the self-assembling building blocks, which is transferred and amplified to the mesoscopic level. A few examples have reported emergence of supramolecular chirality from external stimuli such as light. Here we examine supramolecular chirality of triphenylamine (TPA) derivatives driven by external stimulus, which is circularly polarized light. We will quantitatively investigate their influence on the supramolecular chirality and discuss how supramolecular chirality emerges from different origins.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Investigation of QSPR methods for predicting melting temperature of polymers

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It is necessary to manufacture the polymer material in the desired shape to suit the intended use. The processing temperature of polymer and the state of polymer at specific temperature is one of the most important factors in the development of new polymer material, which is closely related to melting point. However, as the melting point of the polymer can be obtained only through the synthesis of the material and the experiment of the material, it takes a long time to develop a polymer material suitable for the specific purpose. In this study, various QSPR models were developed for the correlation between the structure and melting point of homopolymers and copolymers. Data set of structurally diverse polymers were used to build quantitative structural property relationship (QSPR) models, which were applied in a variety of methods including multiple linear regression, support vector machine, and random forest. The developed QSPR models are suitable solutions to save time and cost by predicting melting point before synthesis and experiment of new polymer materials.

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Poster Presentation : **POLY.P-19**
Polymer Chemistry
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In silico approach for the prediction of surface tension for polymers based on QSPR methods

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As the polymeric material has a multi-phase structure containing one or more interfaces, its surface tension is one of the essential properties in the fields of plastics, elastic bodies, films, fibers and coatings. The purpose of this study is to investigate the tendency of interface to surface tension through chemical structure. We have developed a QSPR (Quantative Structure-Property Relationship) model that predicts surface tension using chemical structures of various homo- and copolymers with surface tension values collected at 25 °C. The algorithms used in this study are multiple linear regression, support vector machine, random forest method. Each model was verified to be a robust and predictive model using bootstrap validation and Y-randomization methods. The developed model helps to reduce the cost and time needed to develop new materials by predicting the surface tension of polymers.

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Poster Presentation : **POLY.P-20**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Zwitterionic Polysulfobetaine Brushes with the Resistance to Nonspecific Protein Adsorption and Platelet Adhesion

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Nonspecific protein adsorption on solid surface leads to platelet adhesion onto the surface. As platelet adhesion anditsexcessive accumulation can cause blood coagulation, the inhibition of platelet adhesion/aggregation has been a critical issue for blood-contact medical devices. For example, unnecessary blood coagulation on vascular stents can lead to blockage of blood flow and blood vessel destruction. In addition, medical devices inserted into the body may lose their function. To solve this problem, we aim to develop the functional coating for preventing platelet adhesion/aggregation by grafting zwitterionic sulfobetaine polymer, poly((3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide) (poly(MPDSAH))onto titanium substrate that is a common material for biomedical applications. The polymerization was carried out by activators regenerated by electron transfer for atom transfer radical polymerization (ARGET ATRP). The polymer grafting process was developed as a substrate-independent manner by using polyphenol chemistry. The polymer grafting was characterized by ellipsometry, contact angle goniometry, and X-ray photoelectron spectroscopy(XPS). The resistance to nonspecific protein adsorption on polysulfobetaine-coated substrate was evaluated by using an enzyme-linked immunosorbent assay (ELISA). Compared to bare and polyphenol-coated substrates, poly(MPDSAH)-grafted substrate strongly inhibited nonspecific fibrinogen adsorption, and platelet adhesion/aggregation, showing its antifouling capability and hemocompatibility

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Mechanical Properties of Low Ion Concentration PSPA Ionomer

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[2]*Department of Polymer chemistry Engineering, Chosun University, Korea*

In this study, a random poly(styrene-co-pentenoic acid) (PSPA) copolymer with 0.7 mol% acid functionality was prepared; the acid groups were completely neutralized with NaOH and $Ba(OH)_2$. The mechanical properties of this ionomer were measured and compared with those of 1.2 mol% poly(styrene-co-acrylate) (PSAA) ionomer. The results showed that the storage modulus of PSPA ionomer was hardly increased, whereas that of PSAA ionomer increased by about 2 times. On the other hand, the T_g of the PSPA ionomer was almost the same as the T_g of the copolymer, but the T_g of the PSAA Na-ionomer was increased by about 3 ℃, and the T_g of the Ba-ionomer was increased by about 2 ℃. This result was probably due to the different distances between the ionic groups and the polymer main chain, which, in turn, affected the multiplet formation and mechanical properties of these two ionomers.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Mechanical Properties of PLA and Random (Styrene-co-sulfonate) Ionomer Blends

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Department of Polymer Science and Engineering, Chosun University, Korea

[1]*Chosun University, Korea*

[2]*Department of Polymer chemistry Engineering, Chosun University, Korea*

In this study, we blended PLA with a random poly(styrene-co-sulfonic acid) copolymer, where the acid groups of copolymer were completely neutralized with NaOH and LiOH, and then examined the mechanical properties of the PLA blend as a function of temperature. The experimental results showed that the glass transition temperature (T_g) of PLA was lowered by 4 ℃ and above T_g the storage modulus was higher when the amount of Li-ionomer in the blend was increased to 20 wt%. However, when the ionomer neutralized with Na was blended with the PLA, the storage modulus and T_g of the PLA were not significantly changed. Therefore, this experiment showed that Li^+ cation of Li-ionomer interacts with the PLA polymer chains through ion-coordination bonds, so Li-ionomer affects the physical properties of PLA. On the other hand, in the case of Na-ionomer, Na^+-sulfonate ion pairs of the ionomer formed strong multiplets, and, thus, the ionomer affected the PLA properties only slightly.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Furanyl-Diketopyrrolopyrrole-Based Chalcogenophene Copolymers with Siloxane Side Chains for Organic Field-Effect Transistors

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[1]*Dongseo University, Korea*

We report the chalcogen atoms effects in organic field-effect transistors (OFETs) by investigating a series of Furanyl-Diketopyrrolopyrrole copolymers (PFDPPF-Si, PFDPPT-Si, and PFDPPS-Si) with different chalcogenophenes commoners (furan, thiophene, and selenophene), where the siloxane-terminated chains are used as solubilizing groups. The optical/electrochemical properties, microstructural analyses, and charge transport characteristics of the resulting copolymers are discussed as a function of the different chalcogenophenes. The larger heteroatom size leads to a bathochromic shift in the absorption profiles and a narrowing of the band gaps. Besides, as the heteroatomic sizes are increased from O, to S, to Se, degree of intramolecular steric hindrance observed in density functional theory calculations follows the trend to deviate from coplanar backbone conformations. Consequently, morphological and crystalline features of PFDPPF-Si are shown to be pronounced high crystalline structure and dense pi−pi stacking, which leads to the achieved best hole mobility of 2.48 cm2 V-1 s-1.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Improvement of Asphaltene Dispersibility by Ionomers neutralized with various cations

Joon-Seop Kim*, **Ki - cheol Song**[1]

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[1]*Department of Renewable Energy Convergence, Chosun University, Korea*

In this study, we investigated how styrene methacrylate (PSMA) copolymers neutralized with various cations affected the asphaltene dispersibility. In order to determine the effects of the type of cations of the ionomers on the dispersibility of asphaltenes, 14.1 mol% PSMA (Mw = 5000) copolymer was synthesized, and the acid groups of the PSMA were neutralized with Na^+, Li^+, and Cs^+. It was found that the dispersibility of asphaltenes by the addition of the ionomers was better than that of the PSMA acid copolymer, regardless of the type of cations. On the other hand, the results also showed that the smaller the size of the cation, the better the dispersibility of asphaltenes.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Dual Cross-Linked Hydrogels That Undergo Structural Transformation via Selective Triggered Depolymerization

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[1]*School of polymer science and engineering, Chonnam National University, Korea*

In this study, we created stimuli-responsive, dual-cross-linked hydrogels that show transformation via selective triggered head-to-tail depolymerization. The hydrogels were established based on aA primary covalent structure containing pendant functional moieties that induce non-covalent interaction with the macro-cross-linker capable of head-to-tail depolymerization. Thus, the incorporation of the macro-cross-linker reinforced the entire structure through physical cross-linking, but, at the same time, the resultant network showed rapid, selective de-cross-linking via the depolymerization reaction, which wholly reverses the chemical structure of material without structural collapse. Furthermore, we used the proposed strategy to design actuating materials that exhibit reversible, programmed, large-scale behavior, and finally demonstrated re-cross-linking by the addition of an extra macro-cross-linker after the de-cross-linking reaction.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Preparation of compressible polymer monoliths that contain mesopores capable of rapid oil–water separation

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This paper describes the design of mesoporous polymer monoliths via a bottom-up approach which are compressible as a biological sponge and provide the rapid separation of oil–water mixtures. The monolithic networks can be prepared in a large scale by a facile condensation polymerization under non-agitated conditions, and contain cyanovinylene repeating units that give rise to a self-assembled fibrous structure and intrinsic mesopores without the need for a template. The sponge-like, polymer network readily absorbed considerable amounts of diverse organic solvents within 60 sec due to the internal designed pores, while excluding water. Most of the absorbates were removed from the wet materials by simply squeezing by hand, and additional washing and drying completely regenerated the original state of materials for reuse. In particular, we observed that the intrinsic mesoporosity enhanced absorption properties of the monoliths when compared with microporous, spongy monolith or melamine foam, and thus demonstrated the rapid, selective separation of a model oil spill under water or on top of water.

Poster Presentation : **POLY.P-27**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

3D Printing Ink Formulation for Soft Matter Photo-Actuator

Monica cahyaning Ratri, Nahee Kim[1], Yeongheon Jung[1], Kwanwoo Shin[1,*]

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Soft actuator, bio-inspired mimicking system is the one of strategy in the medical, soft robotic, pharmaceutical, and tissue engineering[1] due to its dynamic movement toward the presence of external stimuli. By enhancing the additive manufacturing technique and material synthesis, the 3D printed object offers sophisticated and innovative functions such as jumping, complex 3D movement, gripping and releasing. Combination of different formulation of ink, such as active and passive material, can be harnessed to initiate the soft actuator movement expectedly. Poly (N-isopropyl acrylamide) (PNIPAAm) is one of the well-known as active polymers that has temperature sensitive property, shrinking above the lower critical solution temperature (LCST) and swelling below LCST. As a passive material Poly-acrylamide (AAm) combined with alginate has high toughness and elasticity. Due to its surface plasmon resonances (SPR) properties, gold nanorods can absorb light, and release heat to its surrounding [2]. Therefore, the irradiation on the nanoparticle with Near Infrared (NIR) can generate heat locally, and initiate the heat-induced actuation to PNIPAAm containing matrices. We formulated and tested PNIPAAm-metal nanoparticle composites as a bio-ink material to fabricate the heat-sensitive soft actuators for photo-responsive soft robotic motions. In this study, the printability and mechanical properties of the nano-composite bio-ink tested by mechanical measurements, and photo-induced heat responsiveness. We will present our preliminary results how we can formulate the nanocomposite bio-ink, and heat-responsive reactions of the 3D printed soft actuators. Keywords: Soft actuator, PNIPAAm, Gold nanorodsReferences:1.Sydney Gladman A, Matsumoto EA, Nuzzo RG, Mahadevan L, Lewis JA. Biomimetic 4D printing. Nature Materials. 2016;15:413. doi: 10.1038/nmat4544https://www.nature.com/articles/nmat4544#supplementary-information.2.Jana J, Ganguly M, Pal T. Enlightening Surface Plasmon Resonance Effect of Metal Nanoparticles for Practical Spectroscopic Application. RSC Adv. 2016;6. doi: 10.1039/C6RA14173K.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Amino-Functionalized Polymers via Staudinger Reduction

Haeji Jung, Yeong-Gweon Lim*, Sejin Lee

Agency for Defense Development, Korea

The Staudinger reduction, a phosphine-mediated conversion of organic azides to amines, presents an important synthetic method. Since its first report, the Staudinger reduction has found a widespread use in synthetic organic chemistry, materials science and medicinal chemistry. It is also noteworthy that amino groups can be applied to further transformation. In the present work, we report a novel approach for functionalization of azide polymers to amino polymers by Staudinger reduction with triphenylphosphine. We prepared the phenyl-terminated polybutadiene (PtPB) containing azide groups and poly(glycidyl azide polymer) (GAP) as precursors. All of azide groups in polymers converted to amino groups completely with high yields, and products were analyzed for its structural confirmation and determination of important physical and thermal properties.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Polyimide as a functional binder for Ni-rich cathode of high energy Li-ion batteries

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Polyimide has received much attention in the field of electronic materials as a versatile thermo-sable organic material. In this work, the unique combination of nickel-rich NCM811 cathode of Li-ion batteries with functional polyimide binder has been tested to enhanced thermal stability and effective surface passivation in Li-ion batteries, which enables an expansion of electrochemical voltage window to 4.4 V and a flame-resistant cathode. This strategy resolves the issues originating from the interfacial instability of NCM811 cathode coated with conventional binder. As a result, significantly improved cycling stability with higher capacity of than 200 mAh/g is achieved with PI-FTD binder-assisted NCM811 cathode with in commercial liquid electrolyte without any additive. The energy density of 789Wh per kg of cathode active mass delivered by graphite/PI-NCM811 full-cell at 45ºC is 1.5 fold higher than 520Wh per kg of graphite/$LiCoO_2$ commercial LIB. The innovative polyimide binder assisted non-flammable Ni-rich NCM811 cathode concept provides a new direction for ultimately commercially available high energy-density and high-safety Li-ion batteries based on high-voltage and/or high-capacity cathodes.

Poster Presentation : **POLY.P-30**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Donor-Acceptor Random configuration of semiconducting polymer for efficient, flexible and green-solvent processable solar cells

Daehwan Lee, Taewan Kim, Hae Un Kim, Hyuntae Choi, Sungjin Park, Seyeong Lim, Taiho Park*

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

Morphologies and optoelectronic/mechanical properties of semiconducting polymers are significantly affected by their configurations. In this study, thiophene units are introduced into the backbone structure of a semiconducting polymer in either a regular (PffBT-T4) or a random (PffBT-RT4) manner to determine whether the resulting semiconducting polymers are suitable for developing efficient polymer solar cells. The energy levels of both polymers are highly similar because they share the same ratio of sub-units in their backbones however, PffBT-RT4 has lower crystallinity than PffBT-T4 due to its random configuration.Microstructural analyses indicate that PffBT-RT4 exhibits a shorter p–p stacking distance than PffBT-T4. Since short p–p stacking distance benefits interchain charge transport, PffBT-RT4 shows higher space-charge-limited current mobility, and PffBT-RT4 solar cells exhibit higher power conversion efficiency (PCE; 8.84%) than their PffBT-T4 counterparts (7.25%). In addition, PffBT-RT4 solar cells with active layers, prepared using a green solvent without any additive, show an encouraging PCE of 7.23%. Moreover, flexible solar cells based on PffBT-RT4 are much more stable during bending cycles than PffBT-T4 flexible solar cells. Therefore, this study demonstrates that the random configuration approach is a promising design strategy to realize semiconducting polymers for efficient, green-solventprocessable flexible polymer solar cells

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Poster Presentation : **POLY.P-31**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Characterization of Polyurethane Ionomers Based on Pyrrolidinium Ionic Liquids

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Novel polyurethane ionomers are synthesized using dihydroxy functionalized pyrrolidinium ionic liquid, bisphenol-A (or 4,4'-dihydroxybiphenyl, PEG-4000), and 4,4'-diphenylmethane diisocyanate. In order to control the properties of polyurethane, the mole ratio of the ionic liquids and non-ionic diol monoemrs is varied. The polyurethane ionomers are characterized by NMR and FT-IR to see the reaction completions and mole ratio of ionic to non-ionic ratio. The thermal properties of the all polyurethane ionomers are studied by differential scanning calorimetry and thermal gravimetric analysis. Among the polyurethane ionomers with similar chemical structures, Tf_2N^- polyurethanes have higher thermal stability than PF_6^- compounds. The Tf_2N^- polyurethanes are mostly stable up to 300 °C.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

PEG-PA-SC copolymer as polymeric micelle for paclitaxel drug delivery system

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Polymeric micelles consisting of hydrophilic exterior and hydrophobic core have been used widely for delivery of poorly water-soluble drugs. Among these polymeric micelles, the block copolymers are the most commonly used. These amphiphilic block copolymers can spontaneously self-assemble into core/shell nanostructured micelles in aqueous solution at concentrations above the critical micelle concentration (CMC). Due to its self-assembling property, the hydrophobic drugs can be loaded into core of micelle. In this study, poly(ethylene glycol)-poly(D,L-alanine) stearate (PEG-PA-SC) was investigated. Critical micelle concentration and apparent size of micelle are analyzed. Hydrophobic anticancer drug paclitaxel (PTX) is loaded into micelle by solid dispersion method, then loading content and micelle stability are investigated. It is shown that PEG-PA-SC has potentials to be applied as an efficient drug carrier.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Approach to synthesis of peptide mimic antimicrobial polymer using functional glycidyl ether monomer

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

Antimicrobial peptide (AMP) is one of the immune systems contained in many organisms. Most AMPs have a positive charge which interact with the negatively charged bacterial membrane. Also they contain a large amount of hydrophobic amino acid, so they slip into the phospholipid bilayers and destroy their membrane. Because it destroys the membrane directly, bacteria are hard to resist AMPs.Many researchers had synthesized antimicrobial polymers with various backbones using controlled polymerization techniques. However, in many cases, even if the bactericidal effect was high enough, the toxicity was strong, in vivo activity was low, and the biofilm was not successfully removed. To overcome these problems, hydrophilic groups are introduced to control the amphiphilic balance while maintaining bactericidal effect. In addition, the addition of an oligo (ethylene glycol) (OEG) or poly (ethylene glycol) (PEG) side chain with anti-fouling effect can induce the micelle or single chain nanoparticle formation and inhibit protein interaction. Therefore, we synthesized poly (glycidyl ether)s through anionic ring opening polymerization with our functional glycidyl ether monomers - azidobutyl glycidyl ether (ABGE) mimicking lysine with respect to cationic charge, isobutyl glycidyl ether(IBGE) like leucine in terms of hydrophobic groups, and 1-ethoxyethyl glycidyl ether(EEGE) mimicking serine with regard to hydrophilic groups which derived from three most critical active amino acid components - to synthesize polymers with hydrophilic, flexible backbone and various side chains. We expect that it will be useful for the future research of antimicrobial polymers by confirming the characteristics of our polymers compared to other hydrophobic backbone polymers that have been studied so far.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

New Conjugated Copolymer Using Selenophene Monomer and Manufacturing Method, Organic Solar Cell Device Using The New Conjugated Copolymer

Minhyung Kim, Intae Kim*, Eunsang Yu

Department of Chemistry, Kwangwoon University, Korea

In this study, The organic monomers, oligomers or polymers having a conjugated system, that is, a pi-conjugated structure, have been found to have semiconducting properties due to their structural properties, and various studies have been conducted as organic semiconductor materials.On the other hand, group 16 elements, called chalcogen groups, have been applied to various organic materials because of their electronic characteristics. Among them, selenium-containing monomers are relatively studied less than sulfur-containing monomers. Selenium-containing monomers have a low band gap and have the advantage of strong selenium-selenium interactions. In addition, properties such as increased conductivity due to expansion of the conjugation length and wavelength absorption in the near infrared region can be improved, thereby increasing the applicability to the conductive polymer. Therefore, the present study relates to a novel conjugated copolymer having a selenophene monomer, a method for producing the same, and an organic solar cell device using the same. And a technique applied to the organic solar cell device showing a high efficiency by using a different synthesis.Keywords : Chalcogen group, Selenophene, Organic solar cell, Low band gap polymer

Poster Presentation : **POLY.P-35**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and characterization of transparent polyimides derived from 4,4'-oxydiphthalic anhydride, 9,9-bis(4-aminophenyl)fluorene and 2,2'-bis(trifluoromethyl)benzidine

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In this study, we tried creating a new series of the transparent polyimide(PI) films that had more transparent property than previous experimental results. In fact, there have been many researches to develop transparent PIs. But it was not very successful so that in these days many researchers are willing to do a lot of the experiment for developing this way to make transparent PIs. In our research, we synthesized and investigated a PI series using 4,4'-oxydiphthalic anhydride(ODPA) as a dianhydride, and diamine 9,9-bis(4-aminophenyl)fluorene(BAF) and 2,2'-bis(trifluoromethyl)benzidine(TFB) as diamine monomers for increasing transparency. To obtain polyamic(acid) solutions BAF and TFB was used as diamine comonomers, and the ratio of BAF and TFB was adjusted as 8:2, 6:4, 4:6, 2:8, and 0:10 in mole unit. *N*-methyl-2-pyrrolidone(NMP) was used as a polymerization solvent. Then, PI films were fabricated by gradual thermal imidization. The chemical structures of the resulting PIs were characterized by FT-IR spectroscopy and the results well matched as the desired chemical design. The optical properties was recorded by UV-vis spectrometer, The values of λ_{cutoff} of PI films with 20 ㎛ thickness were founded in 431 ㎚, 410 ㎚, 414 ㎚, 420 ㎚, and 408 ㎚ and the values of transmittance at 550 nm were 75%, 92%, 84%, 73% and 86% in the increasing order of TFB, respectively. In addition, thermal properties were investigated by DMA, DSC and TGA. The details will be presented in poster session.

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Microemulsion with near-infrared dye for surface adhesion and photothermal effect

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Department of Chemistry, Pukyong National University, Korea

A highly photostable organic near-infrared (NIR) dye, IR788, converts light to heat. First, IR788-loaded polymer nanoparticles were prepared in aqueous phase to enhance stability and processability. Furthermore, we formulated water-in-oil microemulsion containing the nanomaterials to tune the adhesion property. We believe that the emulsified photothermal agents can be utilized in polar expeditions under sunlight.

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Poster Presentation : **POLY.P-37**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of thiazole derivative bearing thiophene and its electropolymerization and application

Minsub Kim, Intae Kim*

Department of Chemistry, Kwangwoon University, Korea

A thiazole derivative bearing thiophene as a monomer compound was synthesized and electropolymerized at carbon, gold, platinum, and fluorine doped tin oxide electrodes. From an in-depth analysis of cyclic voltammogramsat several scan rates, deposited polymer layers, comprising thiophene functi-onal groups, were shown to clearly exhibit capacitive behavior. This property is related to anion intercalation into these layers during charging and was demonstrated in this study using electrochemical quartz crystal microbalance experiments. It was also shown that in the case of both tetrafluoroborate and hexafluorophosphate anions, the molar ratio of monomers to anions was approx-imately 1:0.6, which is estimated as the ratio of anion intercalation into thiophene moiety of the polymer layers. This confirms that the capacitance p-roperties of these deposited polymer layers have high stability against ele-ctrochemical perturbation. Furthermore, spectroelectrochemistry data obtained during this study indicate that these layers also have switchable electrochr-omic properties in the visible range.Key words : Capacitor, Conducting polymers, Electrochemical quartz crystal microbalance, Electrochomism, Ion intercalation, Spectroelectrochemistry

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

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Electrophoretic determination of aggregation number of Pluronic F127

Naz Fathma Tumpa, Minseok Kwak*

Department of Chemistry, Pukyong National University, Bangladesh

Pluronic F127, poly(ethylene oxide)-b-poly(propylene oxide)-b-poly(ethylene oxide), amphiphilic triblock copolymer can form nanosized micelle in aqueous environment above its critical micelle temperature (CMT) and critical micelle concentration (CMC). Under the condition a defined number of polymer is required to form a spherical micelle, which represents aggregation number (Naggre). in this study, we adopted electrophoresis to determine the Naggre of F127. Micelles consisting of pristine F127 and phosphorylated F127 (PP-F127) were blended in different volume ratio to control the number of surface charges per micelle. Furthermore, the core of micelle was stabilized to prevent exchange of individual polymer among micelles. To assess the role of surface charge coverage on electrophoretic mobility, agarose gel electrophoresis of the blends was performed. By analyzing discrete gel bands, Naggre of F127 we determined was 30.

Poster Presentation : **POLY.P-39**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

3D Printing of Carbon-nanotube/Polydimethylsiloxane Composites for Moldless Flexible Pressure Sensor

Daeyeon Cho, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

due to its broad applications in fields, such as robotics, flexible electronics and medical devices. In compare to traditional sensors, they offer tunable stretch ability and has a high sensitivity. These sensors combine flexible polymers, like PDMS, and nanofillers, like carbon-nanotubes (CNTs), to increase the electrical conductivity of the base polymers. Typically, these nanocomposites have a unique property that change mechanical stimulus to electrical signal. Polydimethylsiloxane (PDMS) is used in a wide range of biomaterial applications including microfluidics, cell culture substrates, flexible electronics, and medical devices. Moreover, it has proved challenging to 3D print PDMS in complex structures due to its low elastic modulus and need for support during the printing process. Carbon-nanotube (CNT) is used in many fields because of its high conductivity. Here, we demonstrate the 3D printing of hydrophobic CNT/PDMS composites within a hydrophilic carbomer gel support via freeform reversible embedding (FRE) to make moldless flexible pressure sensors. In the FRE printing process, the carbomer support act as a Bingham plastic that yields and fluidizes when the syringe tip of the 3D printer moves through it, but act as a solid for the PDMS extrude within it. After we print out CNT/PDMS pressure sensor, we test their mechanical properties, such as conductivity, sensitivity.

Poster Presentation : **POLY.P-40**
Polymer Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Enhancing Resolutuon with One nozzle diameter for Viscoelastic Ink of 3D Bioprinting

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[2]chemistry, Sogang university, Korea

Extrusion based 3D Printing with GelMA(Gelatin Methacrylate), Alginate and Soft hydrogel Inks have difficulties to control degrees of printability and resolution(fiber thickness) to deposit several layers. For making degrees of printability and resolution control of Viscoelastic Inks, I refered 'Harnessing Deformation 3D printing strategy' using One nozzle diameter to control printability and resolution, with various Nozzle speed, Printing height(Nozzle height), Printing pressure for Viscoelastic Inks. GelMA and Geltin/Alginate are generally used for Tissue engineering of 3D Bioprinting, and their mechanical property tunned with concentration, and crosslinking methods. I used mTG(microbial transglutaminase) crosslinked GelMA, enhanced viscosity, and Geltin/Alginate Inks. According to their rheological property, I observed their degrees of printability and resolution(fiber thickness) difference with same parameters. These results can be used more exact resolution for tissue engineering with extrusion based 3D Printing.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

3D printed vascular system with mechanical properties of real blood vessel

Yeongheon Jung, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Despite the significant advancements in bio printing and tissue engineering to mimic native tissue constructs, fabrication of bifurcating vessels and vascularized tissue constructs still pose a great challenge. Previous studies reported various fabricating method of artificial blood vessel which has limitations that control of vessel wall thickness, structural stability, free-standing printed model vasculatures with controlled lumen diameter and wall thickness.The novel method to bioprint bifurcating vessels and develop hierarchical vasculature can overcome the downsides of previous studies. We designed a diffusive bioprinting method by incorporating calcium chloride in Pluronic F127 (PFCa) and casting of alginate/gelatin mixture over the extruded PFCa ink. The rheological properties of PFCa ink is defined. The wall thickness of artificial blood vessel depends on the pressure, nozzle size, incubation time are optimized. Artificial blood vessel, physically modified by acrylate and diacrylate, enables various possibilities of implantation and organ-on-a-chip.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Well-defined Poly(arylene ether sulfone)-b-Polylactide by Chain Growth Condensation Polymerization and Ring Opening Polymerization

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A block polymer consisting of chemically distinctive blocks with high incompatibility can microphase separate at a low degree of polymerization, providing an access to versatile nanostructures at a small length scale below 10 nm features. The high incompatibility characterized by Flory-Huggins interaction parameter (χ) has been achieved by paring polymers prepared by different polymerization mechanisms such as controlled radical polymerization (CRP) and ring opening polymerization (ROP). Recently, we proposed a route to well-defined poly(arylene ether sulfone)-b-polylactide (PES-b-PLA) through combination of chain growth condensation polymerization (CGCP) and ROP. We will present microphase separation behavior of PES-b-PLAs with different molar masses and compositions by small angle X-ray scattering (SAXS) analysis.

Poster Presentation : **POLY.P-43**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Function and oxygen tolerance of initiator-transfer agent-terminator (iniferter) in photomediated reversible addition-fragmentation chain transfer (photo-RAFT)

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Photomediated reversible addition-fragmentation chain transfer (photo-RAFT) polymerization is a practical tool for control the well-defined polymerization under mild condition with the advantages of temporal and spatial control. An innovative point that RAFT agents use as visible light initiator-transfer agent-terminator (iniferter) denotes the polymerization technique without the need for photocatalysts or initiators. However, the research of the comparison of RAFT iniferter polymerization and photoinduced electron/energy transfer (PET)-RAFT polymerization which uses photocatalysts had not been well established. Moreover, each iniferter as RAFT agent show different potential for oxygen tolerance. In this study, we investigated the function of iniferter in photo-RAFT polymerization and compared the abilities of iniferter and photocatalysts in the visible light region, and studied the oxygen tolerance in RAFT iniferter polymerization.

Poster Presentation : **POLY.P-44**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Study of Click Chemistry Reaction on Poly(glycidyl azide-co-tetrahydrofuran) (PGT) with an Alkyne-containing Reactive Energetic Plasticizer and Its Application in Manufacturing Polymer-Bonded Explosives (PBXs)

Mingu Han*, SeungHee Kim

Agency for Defense Development, Korea

We studied azide-alkyne 1,3-dipolar cycloaddition between PGT, prepolymer, and an Prop-2-yn-1-yl-4,4'-dinitropentanoate (PDNP), reactive energetic plasticizer. The conversion efficiency and reaction behaviors depending on the reaction condition, including only heating and a combination of heating and addition of Cu-catalyst, were investigated by an in situ 1H-NMR. And its application as a PGT/PDNP binder system in manufacturing RDX-based PBX was optimized by comparing tensile properties of PBXs formed at different reaction condition.

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Single-Component Organic Solar Cells Materials based on C70-Triads with Controlled Alkyl Chain Spacer

Lim HyoJin, Han Young Woo[*]

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Organic solar cells (OSCs) is promising candidates for flexible and portable device due to their many attractive characteristics such as light-weight and solution-processability. Recently, Outstanding power conversion efficiency (PCE) over 16% has been achieved in bulk heterojunction (BHJ) OSCs consisted of donor (D) and acceptor (A).[1] Single molecular donor–acceptor (D-A) conjugates where the D and A moieties are integrated by a covalent linkage in a single molecule have been reported for its potential as an alternative photovoltaic material.[2] In order to suppress large phase separation in BHJ films, SCOSCs can be a promising strategy. By Incorporating a SC molecule system in OSCs, efficient charge generation in a single molecules and enhanced morphological stability are expected. In this study, we designed and synthesized a new C70-based SC molecule by incorporating different length of alky chain to optimize the morphology and charge transfer characteristics. The detailed synthesis of molecule, optical, morphological, electrochemical and photovoltaic properties will be presented.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Change of Electronic Properties of DPP-Based Small Molecules Depending on Alkyl Chain Position

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

Diketopyrrolopyrrole (DPP) which is a π-conjugated organic semiconducting molecule, is a high performing building block for organic field effect transistors (OFETs). In OFETs devices using a DPP-based material, it shows hole or ambipolar transport characteristics. But n-type has not been developed much compared with p-type due to problems to lower LUMO level. 2-(2,3-dihydro-3-oxo-1H-inden-1-ylidene)propanedinitrile (INCN) is well-known electron acceptor structure. It is a prospective structure that induces deep LUMO level, increases conjugation length, and has efficient intermolecular π-π interactions without distorting the backbone structure. commonly, high-crystalline materials do not dissolve well. This processing trouble can be solved by attaching an alkyl chain of proper length. So, we designed it to have sufficient solubility by attaching an alkyl chain at the INCN group end in different positions. This new INCN moiety was attached to the DPP core to synthesize small molecule, which has high crystallinity without solubility problem and low LUMO level below than -4.0 eV. Finally, an n-type organic semiconductor containing a DPP core shows high electron mobility (~0.8 cm2/Vs).

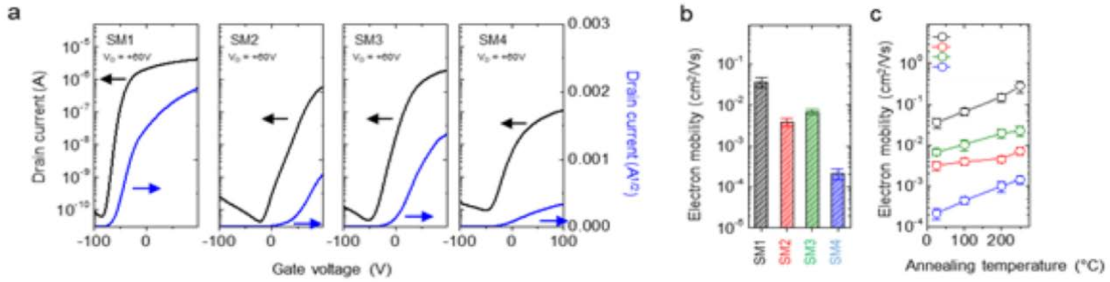

Figure 1. (a) Transfer characteristics. (b) Comparison of electron mobilities of isomers. (c) Variation of the carrier mobilities as a function of the annealing temperature.

Poster Presentation : **POLY.P-47**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Highly conductive and flexible *fluoro sulfonyl imide*-based Single-Ion Conducting Solid Polymer Electrolyte for all solid state Li-ion Battery

Inhwan Choi, Whangi Kim*

Department of Applied Chemistry, Konkuk University, Korea

The polymer lithium ion electrolyte has the advantage of overcoming the safety problem of the organic solvent and can be used even at high temperatures.Among such polymer electrolytes, we synthesized and studied single ion conducting polymer using polyethylene copolymerized polymer.In the case of polyethylene, since the physical flexibility is excellent, film production is easy and the physical stability of the film is high.Due to the high degree of dissociation of Li by the fluorosulfonyl structure, it is possible to achieve high ionic conductivity despite the crystallinity of polyethylene.

Poster Presentation : **POLY.P-48**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Evaluation of Porous Nanoparticles to Improve Hygroscopicity of Fabrics

Eun Ji Park

Advanced material research division, Korea Institute of Footwear & Leather Technology, Korea

Sleeponomics is a compound word of sleep and economics, and the market for sleeponomics is growing at a rapid pace to mitigate the pain and anxiety of people who can't sleep deeply. One of the biggest causes of sleepsleep disturbance is inadequate sleep environment such as light and humidity, and proper sleep environment such as shading and humidity control is an important factor in overcoming insomnia. In this study, we applied porous nanoparticles to the blackout curtains to give them the ability to control the humidity in the room. To solve sleep disturbance, we applied porous nanoparticles to blackout curtains to give them the ability to control indoor humidity. In this study, porous nanoparticles based on silica were prepared. And it was confirmed that the porous nanoparticles were well prepared through the characteristic analysis such as SEM, TEM, FT-IR, NMR in each step.AcknowledgementThis work was financially supported by the Technology Innovation Program (10070125) through the Korea Institute for Advancement Technology(KIAT)

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Formation of Chiral Supramolecules Containing Multiple Hydrogen Bondings

Dong Hwi Kim, **Sang Youl Kim**[1,*]

chemistry, Korea Advanced Institute of Science and Technology, Korea
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Organic compounds containing a TPA moiety can be assembled in chlorinated solvents under light irradiation. Light irradiation generates chlorine radicals that oxidize the TPAs into TPA cation radicals which induce stacking of the TPA molecules. However, it was found that the self-assembled structure didn`t have enough stability at high temperature and showed degradation of chirality as time goes on despite of the photo-polymerization. In this study, TPA derivative having multiple hydrogen bonding sites (TPA-2a-SDA) was synthesized and self-assembled in chlorinated solvents. The chiral supramolecular polymers having improved stability was obtained by self-assembly induced by circularly polarized light (CPL).

Poster Presentation : **POLY.P-50**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Photostable polymeric nanoparticle containing organic near-infrared dye with enhanced biocompatibility under hyperthermal irradiation at low-temperature.

Banyu firdaus Soeriawidjaja, Mingyeong Kang, Hanseong Kim, Minseok Kwak*

Department of Chemistry, Pukyong National University, Korea

Polymeric micelles are versatile nanocarriers to carry hydrophobic molecules within the core in aqueous media. We report engineered polymeric micelles encapsulating highly photostable organic near-infrared (NIR) dye, IR788, for generating heat under NIR irradiation. In addition, the core of micelle is structurally stabilized via *semi*-interpenetrating network formation (sIPN), which ensures stable loading under low temperature and enhances biocompatibility in cell experiment.

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Characterization Polyacrylates Containing Cyclotetrasiloxane for Fouling-Release Coating Applications

Jeong Yong Park, Jong Woon Ha, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

An acrylate monomer containing cyclotetrasiloxane (CTS) were designed and synthesized for anti-fouling coating applications. New acryl-based copolymers consisting of styrene and CTS, poly(styrene-co-CTS)s, were synthesized by changing molar ratios via free radical polymerization. The properties of poly(styrene-co-CTS)s were compared with those of poly(styrene) (PS) as a reference. The content of CTS in the copolymer increased its hydrophobicity also decreased whereas its surface decreased. Protein adsorption studies were conducted to evaluate their fouling-release properties.

Poster Presentation : **IND.P-52**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

MnO2 and banana peel derived porous carbon composites for high performance supercapacitors

Guijun Yang, Soo-Jin Park[*]

Department of Chemistry, Inha University, China

MnO2/biomass-derived porous carbon (BPC) composites have been prepared by a hydrothermal method, in which the BPC 3D porous carbon structure was based on a banana peel. The banana peel, after freeze drying, can maintain its hierarchical natural porous structure, which provides enough growth space for MnO2 and reduces the agglomeration of MnO2 particles. The MnO2/BPC composites were characterized by XRD, FT-IR, XPS, TGA, SEM, TEM, BET. The electrochemical performance of the composites was tested in three-electrode supercapacitors using 1 M Na2SO4 aqueous solution as an electrolyte. Due to the large amounts of hierarchical pores and large pore volume, the as-prepared composites exhibited good electrochemical performance. Electrochemical measurements indicated that the MnO2/BPC composites applied in supercapacitors had a specific capacitance of 139.6 F g-1 at 300 mA g-1, and exhibited a good cycling stability with a capacitance retention ratio of 92.3% after 1000 cycles (at 1 A g-1). The MnO2/BPC composites with 3D porous structure are promising materials in the application of supercapacitors.

Poster Presentation : **IND.P-53**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Li4Ti5O12 anode materials with high specific capacity for lithium-ion batteries

Guijun Yang, Soo-Jin Park[*]

Department of Chemistry, Inha University, China

Li4Ti5O12-y solid solutions were prepared by one-step solid-state carbon thermal reduction reaction. Samples of Li4Ti5O12-y solid solutions are synthesized with different content of carbon black. The presence of carbon black act as reductant. The formation mechanism of Li4Ti5O12 in the presence of carbon (carbon black) was investigated. Moreover, the effect of Ti3+ on the electrochemical performance of the Li4Ti5O12-y solid solutions has been investigated systematically. Among all samples, the sample with 2% carbon black additive exhibited the highest discharge capacity and best cycling stability. Our findings reveal that the surface modification with carbon black can improve the electrical conductivity and Li+ diffusion coefficient and improve rate capacity and cycling stability significantly.

Poster Presentation : **IND.P-54**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of carbon-based NiCo2O4 as electrodes for an asymmetric supercapacitors

Guijun Yang, Soo-Jin Park*

Department of Chemistry, Inha University, China

We demonstrate a simple hydrothermal approach to obtain a carbon-based NiCo2O4 material for use in supercapacitors. In this process, filter paper was submerged in a NiCo2O4 precursor solution, and the final product was obtained after calcination in an Ar2 atmosphere. The hydroxyl group-containing cellulose in the filter paper facilitates the formation of 3D structures, which not only improve the electrical conductivity but also provide fast electron and ion transport after calcination at high temperature, thus improving the electrochemical performance. An asymmetric supercapacitor has been assembled by using NCO/C-2 and activated carbon as the positive and negative electrodes. The NCO/C-2//AC ASC device exhibits a maximum energy density of 20.87 Wh kg-1 at a power density of 374.6 W kg-1 and a maximum power density of 7.48 kW kg-1 at an energy density of 11.43 Wh kg-1.

Poster Presentation : **IND.P-55**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Effect of N-doped TiO_2/g-C_3N_4 composites for enhanced visible light photocatalytic activity.

SeongJun Mun, Soo-Jin Park[1,*]

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

Composites consisting of N-doped TiO_2/g-C_3N_4 were prepared using the sonochemical synthesis and hydrothermal method. Structural properties of the composites were characterized by X-ray diffraction spectroscopy (XRD), X-ray photoelectron spectroscopy (XPS), UV-vis diffuse reflectance spectra (UV-vis DRS) and scanning electron microscopy (SEM) transmission electron microscopy (TEM). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of N-doped TiO_2/g-C_3N_4 composites were improved compared to pure TiO_2. The results indicated that reduced g-C_3N_4 band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-56**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Effect of Pt-loaded g-C_3N_4/TiO_2 nanofibers for Enhanced visible light photocatalytic activity via electrospinning

SeongJun Mun, **Soo-Jin Park**[1,*]

Inha University, Korea

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

The of Pt-loaded g-C_3N_4/TiO_2 nanofibers were prepared via electrospinning and hydrothermal method. The as-prepared composite photocatalysts were characterized by X-ray diffraction (XRD), Raman, scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS) and UV-vis diffuse reflectance spectra (UV-vis DRS). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of Pt-loaded g-C_3N_4/TiO_2 nanofibers were improved compared to pure TiO_2. The results indicated that reduced Pt-loaded g-C_3N_4 band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-57**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Highlighting the role of ultra-micropores for CO2 and methylene blue adsorption

Adeela Rehman, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Microporous carbons synthesized from sucrose and melamine in the presence of molten salts present a facile strategy to design high micropore content in the carbonaceous materials. Series of nitrogen-doped samples were prepared by changing the ratio of melamine to sucrose from 0 to 2. The optimized material possesses excellent textural features, narrow micropores and high micropore volume (

Poster Presentation : **IND.P-58**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Delineating the role of heteroatoms in CO2 adsorption

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Microporous carbon materials are envisaged as efficient contenders for mitigating CO2 level and global climate change by virtue of their rich surface chemistry, high specific surface area, tunable pore structures, moderate heat of adsorption, and facile regeneration. Current work presents a solvent-free activation approach for designing a series of microporous carbons using economically favorable avenue. Synthesized carbon materials possess a high surface area, large pore volumes, and hierarchical meso-micro and ultramicroporous structures. The high adsorption capacities with the facile regeneration make these microporous carbons amongst the most promising adsorbents in clean energy and environmental applications.

Poster Presentation : **IND.P-59**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Carbon capture by nitrogen-enriched microporous carbons

Adeela Rehman, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

The construction of physical or chemical adsorbents for CO2 capture and sequestration (CCS) is a vital technology in the interim period on the way towards a sustainable low-carbon future. The search for efficient materials to satisfy the increasing demand for CCS has become extremely important. On account of the dipole–quadrupole interactions between the polarizable CO2 molecule and the accessible nitrogen site, the investigations have indicated that the incorporation of accessible nitrogen-donor groups into the pore walls of porous materials can improve the affinity to CO2 and increase the uptake capacity and selectivity. Hence, nitrogen-rich porous materials as highly promising CO2 adsorbents have been broadly fabricated and intensively investigated.

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Poster Presentation : **IND.P-60**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of PIBSI derivatives with heterocycles containing S and N and friction reducing effects

Joonho Kim, Yeong-Joon Kim*, Jaehee Song[1]

Department of Chemistry, Chungnam National University, Korea
[1]*Department of Chemistry, Suncheon National University, Korea*

HRPB350 and HRPB260 were synthesized by cationic polymerization. Polyisobutenyl succinic anhydride (PIBSA) was synthesized by the reaction of HRPB350/ HRPB260 and maleic anhydride and then converted to polyisobutenyl succinimide (PIBSI) derivatives by introducing heterocyclic moieties. The new PIBSI derivatives were expected to act as friction reducing agents since these molecules contain S and N which strongly interact with metal surfaces. The structures of PIBSI derivatives were confirmed by NMR and MALDI-TOF. The wear scar diameter (WSD) in Yubase 6 and DB51 base oil was measured using a 4-ball tester. The wear scar diameters with 1 % polyisobuteneyl succinimide (PIBSI) additives are comparable to those with commercially available products

Poster Presentation : **IND.P-61**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Hydrogen storage in porous carbons form silica-eliminated coconut shells at low temperature and high pressure

Ji-Hye Park, Soo-Jin Park[1,*]

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

In this work, silica elimination and chemical activation were carried out using potassium hydroxide, which gave a potential for various porosity. The morphologies of ACs were observed by scanning electron microscopy (SEM). For elemental analysis of surface, Energy dispersive X-ray spectroscopy (EDS) was used to analyze the composition of sample surface. The specific surface area and pore size distribution were calculated by N_2/77 K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were obtained by high pressure adsorption instrument at 77 K and 60 bar.

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Poster Presentation : **IND.P-62**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Hydrogen storage capacity of activated carbons from coffee wastes

Ji-Hye Park, Soo-Jin Park[1,*]

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

In this work, activated carbons (ACs) were synthesized using KOH activation with various temperatures. X-ray diffraction (XRD) was conducted to investigate structural properties of ACs. Scanning electron microscopy (SEM) observed the morphology of ACs. The N_2/77 K adsorption isotherms were used to obtain the specific surface area and pore size distribution using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen adsorption isotherms were measured by high pressure adsorption system at 298 K and 20 bar. The results suggest that the temperature for KOH activation would affect on porosity and hydrogen uptakes.

Poster Presentation : **IND.P-63**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Improvement of Properties and Processes of Cyanoacrylate based UV Absorbers with Methoxy Substituent

JoungJin Im, Won Ki Lee[1], Youngeup Jin[2,*]

Industry chemistry, Pukyong National University, Korea
[1]*Department of Polymer?Engineering, Pukyong National University, Korea*
[2]*Engineering Chemistry, Pukyong National University, Korea*

As the weather changes due to the recent environmental pollution caused by industrial development, corrosion and aging of products are accelerated by various polymers exposed to the outside. Ultraviolet rays are the cause of promoting decomposition of such polymers. Ultraviolet rays are mainly strong in the equatorial region with a lot of insolation, and ultraviolet rays are classified into UVA, UVB, and UVC depending on the wavelength. In this study, acrylic cyanate-based products are synthesized environmental friendly UVA by improving quality and yield. Various substituents including electron donating substituents versus electron withdrawing substituents, methyl and phenyl groups were compared. This led to the introduction of methoxy substituents for comparison and analysis as the most potential substances in terms of physical properties and ecomonics. Due to this, methoxy substituent was introduced for comparison and analysis as the most potential material in terms of physical properties and economics. The process conditions (temperature, catalyst, solvent) of each synthesis method were changed to optimize the process to obtain high yields. As a results P-E was achieved UV absorbance of 88.5% in 337nm, color of solution of 66.1% in 460nm and 98.2% in 500nm, and heat stability of 25%.

Poster Presentation : **IND.P-64**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Eco-friendly Process Improvement without Using Toluene of Acrylic cyanate UV Absorber with Fluorine Substituent

Sanghun Ahn, Won Ki Lee[1], Youngeup Jin[2,*]

Pukyong National University, Korea
[1]*Department of Polymer?Engineering, Pukyong National University, Korea*
[2]*Engineering Chemistry, Pukyong National University, Korea*

Recently, as interest in environmental problems and health has increased, interest in ultraviolet rays has gradually increased. The property degradation reaction of ultraviolet rays reached through the atmosphere is a reaction proceeding in the presence of oxygen in the air and is an oxidation reaction initiated by ultraviolet rays. It causes color change and peeling phenomenon such as display, composite material and automobile industry, and causes many side effects. To solve this problem, UV absorbers are developed to absorb rays and release them as thermal energy. This study deals with cyanoacrylate UV absorbers and basically removes ammonia from the process to practice eco-friendly process. In order to compare and analyze the electron donor substituents and the electron withdrawing substituents, the fluorine derivatives having the best physical properties were synthesized and analyzed. Since toluene was not used during the whole synthesis process, it was environmentally friendly. The process conditions (temperature, catalyst, solvent) of each synthesis method were changed to optimize the process to obtain high yields. As a results P-H was achieved UV absorbance of 77.6% in 317nm, color of solution of 97.5% in 460nm and 99.5% in 500nm, and heat stability of 93.5%.

Poster Presentation : **IND.P-65**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Modification of pristine titanium oxide materials for lithium adsorption and desorption

Urooj Kamran, Soo-Jin Park[1,*]

Inha University, Korea

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

In this research, the adsorption potential of lithium ions (Li+) by pure titanate nanotubes (TNTs) functionalized TNTs was examined. We used simple hydrothermal method for fabricating TNTs at 130 oC and these synthesized TNTs were functionalized by different OCs including urea, melamine and polyacrylonitrile using titanium (IV) oxide powder as a precursor via impregnation approach. The crystallinity, morphology and functional group properties of prepared adsorbents were characterized. The Li+ adsorption mechanism considered as an ion exchange reaction among Li+ ions and ions exist in an interlayer of pure and functionalized TNTs. Different kinetic models have applied on equilibrium experimental data to determine the rate and nature of adsorption process. The recovery of Li+ ions was done by using hydrochloric acid as an extracting agent with three repeated cycles.

Poster Presentation : **IND.P-66**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Influence of Nickel contents on MnO2 nanoparticles decorated on rGO sheet for Lithium adsorption and recovery

Urooj Kamran, Soo-Jin Park[1,*]

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

The weight ratios controllable synthesis of novel and effective RGO-Nix/MnO2y nanocomposites was done by hydrothermal approach. The reduction of graphite to graphene oxide, fabrication of MnO2 and deposition of Ni-MnO2 above the surface of reduced graphene oxide was individually carried out by hydrothermal technique. The physical and morphological properties of prepared nanocomposites was analyzed. The batch adsorption experiment was performed to identify the lithium uptake capability of nanomaterials, in this study following parameters optimized to enhance adsorption rate; including effect of pH, dosage, contact time, and preliminary Li+ solution concentrations. The various kinetics and equilibrium isothermal models applied on experimental data to identify the nature of adsorption phenomena. To make process more economic and efficient, the Li+ desorption experiment performed. Briefly, it can be concluded that the prepared nanocomposites possessed adequate potential for lithium uptake.

Poster Presentation : **IND.P-67**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Role of Nickel ratio in MnO2/graphene oxide hybrid as an adsorbent for Lithium capture and recovery

Urooj Kamran, Soo-Jin Park[1,*]

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

A novel and effective RGO-Nix/MnO2y nanocomposites was done by hydrothermal approach. The reduction of graphite to graphene oxide, fabrication of MnO2 and deposition of Ni-MnO2 above the surface of reduced graphene oxide was individually carried out by hydrothermal technique. The physical and morphological properties of prepared nanocomposites was analyzed. The batch adsorption experiment was performed to identify the lithium uptake capability of nanomaterials, in this study following parameters optimized to enhance adsorption rate; including effect of pH, dosage, contact time, and preliminary Li+ solution concentrations. The various kinetics and equilibrium isothermal models applied on experimental data to identify the nature of adsorption phenomena. To make process more economic and efficient, the Li+ desorption experiment performed.

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Poster Presentation : **IND.P-68**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Effect of porosities and surface characteristics on polythiophene-derived carbons for lithium ion recovery from sea water

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, the sulfur (S) -doped porous carbons (PCs) were derived from polythiophene (PTh) as a S-riched carbon precursor and prepared by chemical activation with potassium hydroxide (KOH). The lithium adsorption experiments were carried out to analyze the influence of porous texture properties changed by the chemical activation of PCs on adsorption rate. From the experimental results, it was observed that the extent of adsorption process depends on the sulfur (S) and oxygen (O) group increases. Consequently, it could be noted that lithium ion recovery behaviors are greatly influenced by the surface functional groups and textural properties of PCs surfaces, resulting in enhanced electron acceptor-donor interaction at interfaces.

Poster Presentation : **IND.P-69**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of amine-modified titanate nanotubes for CO_2 capture under flue gas condition

Young-Jung Heo, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Amine-modified adsorbents have been of interest due to their excellent performance for carbon dioxide (CO_2) capture. In this work, we have prepared titanate nanotubes (TNTs) with amine modification using polyethylenimine (PEI) for selective CO_2 capture under flue gas. TNTs were prepared by the hydrothermal reaction, and PEI-functionalized TNTs (P-TNTs) were prepared by the wet impregnation method. Enhanced CO_2 affinity through amine modification on TNTs allows for selective and favorable CO_2 adsorption onto adsorbents. To confirm the CO_2 capture in the post-combustion step, CO2 adsorption performances were investigated by the gravimetric method under 15% CO_2 /85% N_2 (binary) and 15% CO_2/5% O_2/80% N_2 (ternary) gases as in flue gas conditions, respectively. Furthermore, our work provides evidence that the amine-modified adsorbents can be influenced by oxygen gas on CO_2 capture performances, including regeneration ability.

Poster Presentation : **IND.P-70**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A study of controlling pore size on carbon aerogels using physical activation for efficient hydrogen storage and supercapacitor applications

Young-Jung Heo, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, carbon aerogels (CAs) were prepared as physisorbents and electrode materials for hydrogen (H2) storage and supercapacitor. Synthesized aerogels were carbonized and then activated using carbon dioxide (CO2) gas. The specific surface area and micropore size distribution were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and non-linear density functional theory method. The structural and morphological properties were investigated by X-ray diffraction (XRD) and scanning electron microscope (SEM), respectively.The hydrogen uptakes were analyzed at 77 K and 1 bar. Electrochemical behaviors were investigated by cyclic voltammetry (CV) in a three-electrode system. From the results, it was found that surface characteristics and porosities played an important role in the capacitance of electrode and hydrogen uptakes.

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Poster Presentation : **IND.P-71**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Research trends and chemical approaches in seawater desalination

Jae Young Ha

Department of Chemistry, Hankuk University of Foreign Studies, Korea

According to recent media, about 1 billion people worldwide suffer from water shortages. About 70% of the earth's surface is water, but less than 3% of our freshwater is available. In addition, according to the UN report, by 2030, demand for water will exceed 40% of supply due to climate change and population growth. In order to solve such a water shortage phenomenon, various studies are being conducted, one of the most common solution is seawater desalination technology. This study summarizes the chemical approach of recent seawater desalination technology and examines its advantages and disadvantages. It also examines recent research trends for each technology and predicts and suggests future directions for future research.

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Poster Presentation : **IND.P-72**
Industrial Chemistry
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Influence of amino-functionalized MoS2 nanosheets on fracture toughness and thermal stability of epoxy nanocomposites

Shahina Riaz, **Soo-Jin Park**[1,*]

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

In this study, branched polyethyleneimine (b-PEI)-assisted exfoliation of MoS2 nanosheets (MoS2¬-PEI) was carried out. These non-covalently functionalized MoS2-PEI nanosheets were employed as toughening agents for epoxy composites. The contents of MoS2-PEI nanosheets were maintained at weight fractions lower than 0.16 wt%. The epoxy composites exhibited a 67% increase in fracture toughness (KIC) and a corresponding 101% increase in fracture energy (GIC) at nanosheets loadings as small as 0.06wt.% (MP-6), KIC shows linear relationship with the surface free energy (SFE) and is highest at 81 mJ m−2 for the MP-6 composite. The overall flexural modulus (E) and strength (σ) were not highly responsive to the addition of the MoS2-PEI nanosheets. Furthermore, the thermal stability of the epoxy composites improved significantly. The optimum MoS2-PEI nanosheet loading was observed to be 0.06wt.%, beyond which a gradual decrease in the thermal stability was observed.

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Poster Presentation : **IND.P-73**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Fracture toughness of epoxy nanocomposites filled with melamine functionalized WS2 nanosheets

Shahina Riaz, **Soo-Jin Park**[1,*]

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

In this work, a melamine functionalized tungsten disulfide nanosheets (M-WS2) were fabricated and used as fillers to form epoxy EPR/M-WS2 nanocomposites. The effects of WS2 and M-WS2 loadings on the mechanical properties of epoxy composites were investigated and compared. With only addition of 0.5 wt% M-WS2, the fracture toughness (KIC) and fracture energy (GIC) of EPR/M-WS2 nanocomposites showed 68% and 94% improvement over the neat epoxy. Interestingly, the flexural modulus and strength of EPR was also increased with the introduction of M-WS2 fillers. These properties could result from the good dispersion and strong interfacial adhesion of M-WS2 fillers and the EPR matrix. Therefore, this work provides a facile way to produce of high-performance EP nanocomposites.

Poster Presentation : **IND.P-74**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Non-radiative decay and Photophysical Investigation of Ir(III) Dopants with *N*-heterocyclic carbene ligands: Geometries, electronic structure, and blue PHOLED device performance

Bo-Sun Yun, Su-Jin Kwak, Changhyun Back, Min Su Choe, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

To develop new type of Ir(III) complexes as a blue-phosphorescent dopant in the organic light-emitting diode (OLED) devices, we designed C^C-coordinated N-heterocyclic carbene Ir(III) complex isomers (fac-IrSiPr (**f-IrSiPr**), mer-IrSiPr (**m-IrSiPr**) and mer-IrSMe (**m-IrSMe**). The single-crystals of **f-IrSiPr** and **m-IrSiPr** were analyzed to get the structural information by X-ray crystallography. The **IrS** showed the blue phosphorescence at around 450 nm at 300 K, which were slightly red-shifted with increasing solvent polarity. At 77 K, the emission spectra showed the small rigidochromic shifts of ca. 4 nm. Density functional theory (DFT) was applied to study the molecular structure, the energy level, and the orbital distribution. Time-dependent DFT calculation also performed to assign the optical transitions. The radiative rate constant (k_r) and non-radiative rate constant (k_{nr}) were determined using the emission quantum yields and the lifetime data. The k_r values were independent of temperature, but the k_{nr} values varied inversely with the temperature rising. The activation energies for k_{nr} were determined in the range of 1012–1447 cm^{-1}, which are too low energy to access the metal-centered state. Therefore, we suggested that the main deactivation pathway is attributed to intrinsic low-energy vibration motions and solvent nature. We fabricated the OLEDs devices using **m-IrSiPr** and **m-IrSMe** as a dopant in the solution process. The OLED devices showed the blue electroluminescence, which was investigated in terms of the current density-voltage-luminance (J-V-L), the current efficiency, the power efficiency, and the external quantum efficiency.

Poster Presentation : **IND.P-75**

Industrial Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Development of highyl efficient deep blue Phosphorescent Ir(III) dopant through incorporation of an electron-withdrawing -SO_2CF_3 substituent to cyclometalating C^N-phenyl pyridine (ppy)

Jin-Hyoung Kim, Su-Won Na, Daehan Lee, Jeong-Wan Yu, Dae won Cho*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Incorporation of an electron-withdrawing -SO_2CF_3 (σ_p = 0.96) substituent in cyclometalating C^N-phenyl pyridine (ppy) ligand resulted in an expected blue-shifted phosphorescence derived from homoleptic Ir(C^N)$_3$ complexes [λ_{em} = 457 nm for **Ir(ppySCF$_3$)$_3$** at 77 K]. Its heteroleptic counterpart, modified by a pyrazolyl borate LX ligand, **Ir(ppySCF$_3$)$_2$(bor)** exhibited further blue-shifted phosphorescence (λ_{em} = 455 nm at 77 K). Density-functional theory (DFT) calculations supported the efficacy of electron-withdrawing capability of the SO_2CF_3 substituent lowering HOMO energy and obtained a widened band-gap and resumed a deep blue emission. Stronger σ-bond of C_{Ph}-Ir correlates well to a higher emission quantum yield of **Ir(ppySCF$_3$)$_3$** than that of **Ir(ppySF)$_3$**, the reported fluoro sulfonyl (-SO_2F) derivative which is devoid of a ^{3}MC deactivation manifold resulting in the quantum yields (Φ_{PL}) of **Ir(ppySCF$_3$)$_3$** and **Ir(ppySF)$_3$** to be 0.89 and 0.72, respectively. Finally, among solution processed multilayered devices having an ITO/PEDOT:PSS/TCTA:Ir dopants (10:1, *w*/*w*)/TmPyPB/Liq/Al structure, a heteroleptic dopant, **Ir(ppySCF$_3$)$_2$(bor)**, exhibited a better device performance reporting an external quantum efficiency (EQE) of 1.14%, current efficiency (CE) of 2.31 cd A^{-1}, and power efficiency (PE) of 1.21 lm W^{-1} together with a blue chromaticity CIEx,y = 0.16, 0.32.

Poster Presentation : **IND.P-76**
Industrial Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Home-built solid-state NMR probes for many static samples

Ji-Ho Jeong, Yongae Kim*

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Solid-state NMR has seen a constant increase in popularity since the NMR had been first invented because it hurdled the biggest problem; inherent lack of resolution relative to solution-state NMR; with many techniques. Solid-state NMR serves many insights for organic and inorganic chemistry, where is used as a powerful tool to study local dynamics, kinetics as well as thermodynamics of a variety of systems. Many factors of each NMR assembly determine the performance of the NMR spectroscopy. Especially, the probe is the interface between a sample and the spectrometer. Its high solidity and flexibility are very important elements for supporting the maximum performances of the NMR spectrometer. Above all, the choice of a probe suitable for various types of samples is needed for getting the right results from NMR experiments. So we made the elaborate solid-state NMR probes for diverse sample analysis such as characterizing membrane proteins and defining of molecular dynamics in high tech devices. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) & narrow bore (NB) 1H-15N double-resonance NMR probe and a home-built 800 MHz NB 1H-15N NMR probe for biological samples. For the study of the mode of action of an antimicrobial peptide, we made 400 MHz 1H-31P double resonance NB probe. We will also announce a home-built 400MHz and 500 MHz NB 19F-13C NMR probes for analyzing nano-materials and LCD panel respectively and 600 MHz NB 19F-7Li NMR probes with a 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.

Poster Presentation : **INOR.P-1**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Selective Nitric Oxide Transmission in Cell Signaling by Using a Photodegradable Cobalt(III)-Nitrosyl Complex

Jisu Choe, Jaeheung Cho[1,*]

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[1]*Emerging Materials Science, DGIST, Korea*

Cells use enzymatically synthesized gaseous molecules such as nitric oxide (NO) to transmit both of intracellular and intercellular signals.Although these enzymatically and endogenously synthesized gaseous molecules can be used to precisely regulate physiological changes in the cells, tissue, or organisms, difficulties in overcoming random diffusion have made the development of chemical delivery tools with fine temporal resolution has been elusive. To address this challenge, we synthesized a photo-cleavable metal-nitrosyl complex, $[Co^{III}(MDAP)(NO)(CH_3CN)]^{2+}$ (MDAP = *N*,*N*'-dimethyl-2,11-diaza[3,3](2,6)pyridinophane), which can stably deliver and selectively release NO in the cytosolic region. It has been characterized by crystallographic and spectroscopic methods and it releases NO with a high quantum efficiency ($\Phi_{NO} = 0.78$) in H_2O, upon activation with light. Theoretical calculations support our interpretation that the dissociation of NO occurred in the singlet excited state. We demonstrate its utility by researching the extracellular signal–regulated kinases (ERKs). By observing the dynamics of ERK responses using a kinase translocation reporter (KTR), we showed how the cells use both exogenous and endogenous NO to classify cellular responses. Using this technique, we can understand how various cellular signaling networks are dynamically interconnected and regulate drug delivery pathways.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Nucleophilic Reactivity Difference between Macrocyclic and Open-Chain Nickel(III)-Peroxo

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A peroxonickel(III) complex bearing the Me_6-trien ligand, an open-chain analogue of the macrocyclic 12-TMC ligand, was synthesized and characterized by several physical methods, such as UV-vis, resonance Raman, ESI-MS and EPR. Density functional theory calculations provide geometric and electronicconfigurations of peroxonickel(III) complexes. The reactivity of the peroxonickel(III) intermediate wasexamined in oxidative nucleophilic reactions (e.g., aldehyde deformylation). By comparing the reactivitiesof the open-chain and macrocyclic peroxonickel(III) complexes under identical reaction conditions, wewere able to demonstrate that the open-chain peroxonickel(III) complex is much more reactive than themacrocyclic analogue in aldehyde deformylation. This result provides intriguing aspects of the reactivitydifferences for open-chain vs. macrocyclic systems of metal complexes.

Poster Presentation : **INOR.P-3**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Polydiacetylene Loaded with Metal Complexes for Visible-Light-Driven Photocatalytic NADH Regeneration and CO2 Conversion

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[1]*ChemistryNanoscience, Ewha Womans University, Korea*
[2]*Ewha Womans University, Korea*
[3]*Chemistry, Ewha W. Univ., Korea*

Artificial photosynthesis can convert the solar energy into the solar fuel such as hydrogen by driving high-energy chemical reactions. To fabricate artificial photosynthetic systems, efficient visible light-absorbing materials have to link reduction and oxidation catalysts for an efficient energy flow. As a step toward this goal of an NADH regeneration system and enzymatic production of solar fuels from CO2, we studied the synthesis of a new conjugated polydiacetylene polymer that is covalently connected with [Ru(phen-NH2)(bpy)2]2+. The [(bpy)2Ru(phen)]-polydiacetylene absorbed a wide range of visible light because of the presence of two chromophores, the Ru complex and polydiacetylene. The electron transfer from the photoexcited [Ru(phen)(bpy)2]2+ to the polydiacetylene backbone was observed. In a visible light-driven photocatalytic NAD+ reduction by (cyclopentadienyl)Rh(bpy)(H2O)2+ with [(bpy)2Ru(phen)]-polydiacetylene, NADH was regenerated. The consecutive carbon dioxide reduction coupled with formate dehydrogenase was carried out to utilize the photoregenerated NADH catalytically. To understand the mechanism of the photochemical reactions with Ru- or Rh-loaded PDA, picosecond transient absorption and emission spectroscopy are used.

Poster Presentation : **INOR.P-4**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Electrochemical Oxidation of Guanines of DNA Loaded on Reduced Graphene Oxides

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Studing the interactions of biomolecules DNA/RNA with carbon nanomaterials is very important for applications in bioassay and bioanalysis. Graphene and graphene oxide (GO) have been successfully adopted by exploiting the binding affinity difference between single-stranded oligonucleotides (ssDNA) and double-stranded oligonucleotides (dsDNA) to graphene sheets. In this work, we describe the electrochemical DNA oxidation with [Ru(bpy)3]2+ to understand the interaction between dsDNA (and corresponding ssDNA) and reduced graphene oxide (rGO). The electrochemical oxidation rate of guanine bases of ssDNA bound to rGO by electrochemically generated [Ru(bpy)3]3+ was much slower than that unbound to rGO. Our study revealed that ssDNA constrained on rGO was significantly protected from the electron transfer to [Ru(bpy)3]3+ because of π,π-stacking interaction between nucleobases and rGO. On the other hand, the oxidation rates of 11-, 20-, and 27-mer dsDNA bound to rGO increased relative to those of dsDNA alone, demonstrating that the guanine bases of dsDNA on interacting with rGO became more accessible to [Ru(bpy)3]3+. Our electrochemical data illustrated that dsDNA could be totally or partially dehybridized and bind to rGO to form ssDNA/rGO. Furthermore, absorption, circular dichroism spectra, and fluorescence measurements of ethidium bromide using ssDNA and dsDNA with rGO supported the dehybridization of dsDNA in the presence of rGO.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and properties of (phosphine)gold azides

Heekwon Park, MinGyu Ham, Yong-Joo Kim*

Department of Chemistry, Kangnung-Wonju National University, Korea

Gold azides have been attracted as useful precursors for heterocycle formation or bioactive materials. In this work, various (phosphine)gold azides, Me_3PAuN_3, Et_3PAuN_3, (dppm)$(AuN_3)_2$ and (dppf)$(AuN_3)_2$ were prepared from treatments of corresponding chlorides with aqueous NaN_3. Reactions toward organic isocyanide (R-NC) and isothiocyanates (R-NCS) were examined and detail explanation will be discussed.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Overview of Chemical Crystallography Beamline in Pohang Light Source II

Dae-Woong Kim, Dohyun Moon*

Beam Operation Team, Pohang Accelerator Laboratory, Korea

The unique chemical crystallography beamline exists in Pohang Light Source II. It is dedicated crystallography beamline for the structure solution of crystalline materials both small and supramolecule using synchrotron X-ray radiation. The beamline is located at the 2D bending magnet port in the 3 GeV storage ring (400mA, Top-Up mode) of Pohang Light Source II. The diffraction data are collected by newly installed a Rayonix MX225HS CCD area detector with high precision goniostat. These equipment combinations are delivered to get the high-resolution diffraction image and extremely fast data collection. The tunable energy range between 8 and 20 keV (1.5 and 0.6Å) is supplied by a Si(111) double crystal monochromator and controlled by users on demand. The beamline control and data collection are controlled by custom-made BL2D-Supramolecular Data Collection Software (BL2D-SMDC). The software has an interactive Windows GUI and is designed to run on a user-friendly. The HKL3000sm software is used for indexing, integration, and scaling. The instruments status and various application using beamline will be presented in this poster.

Poster Presentation : **INOR.P-7**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

A Mononuclear Nonheme Chromium(V)–Oxo Complex and Its One-Electron Oxidized Species

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A mononuclear chromium(V)–oxo complex with tetraamido macrocyclic ligand (TAML), $[\mathrm{Cr^{V}(O)(TAML)}]^{-}$ (**1**), was synthesized and characterized structurally and spectroscopically by X-ray, UV-vis, EPR, CSI-MS, and rRaman. In hydrogen atom transfer (HAT) and oxygen atom transfer (OAT) reactions, **1** was a sluggish oxidant in the absence and presence of $\mathrm{Sc^{3+}}$ ion. One-electron oxidized species of **1**, $[\mathrm{Cr^{V}(O)(TAML^{+\bullet})}]$ (**2**), was also synthesized by reacting **1** with $[\mathrm{Ru^{III}(bpy)_3}]^{3+}$ (3 equiv.) in the presence of $\mathrm{Sc^{3+}}$ ion and characterized spectroscopically. Formation of **2** was also confirmed by spectroelecrochemistry. As shown in Cpd I and Cpd II in heme systems, chromium(V)–oxo TAML cation radical species **2** was much more reactive than **1** in HAT and OAT reactions. For example, although **1** was unreactive with thioanisole in the presence of $\mathrm{Sc^{3+}}$ ion even at room temperature, **2** reacted extremely fast with thioanisole even at –40 $^{\circ}$C, indicating that **2** is an active oxidant in HAT and OAT reactions.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and Structural Characterization of Cadmium(II), Cobalt(II), Copper(II) and Zinc(II)Complexes Containing 4,4'-Oxybis-*N*,*N*-bis((1H-pyrazol-1-yl)methyl)aniline

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We have synthesized a series of cadmium(II), cobalt(II), copper(II) and zinc(II) complexes by the reaction of ligand 4,4'-oxybis-*N*,*N*-bis((1H-pyrazol-1-yl)methyl)aniline (L_{OBPA}) with **[$CdBr_2\cdot4H_2O$]**, **[$CoCl_2\cdot6H_2O$]**, **[$CuCl_2\cdot2H_2O$]**, and **[$ZnBr_2$]** in ethanol, respectively. The corresponding dinuclear complexes, [(L_{OBPA})Cd_2Br_4], [(L_{OBPA})Co_2Cl_4], [(L_{OBPA})Cu_2Cl_4], and [(L_{OBPA})Zn_2Br_4] were characterized by IR, ^{1}H-NMR, ^{13}C-NMR, elemental analyzer, and X-ray single crystal diffraction. Specifically, molecular structure of [(L_{OBPA})Co_2Cl_4] and [(L_{OBPA})Zn_2Br_4] were distorted tetrahedral geometry around metal center. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of MeLi were investigated at room temperature.

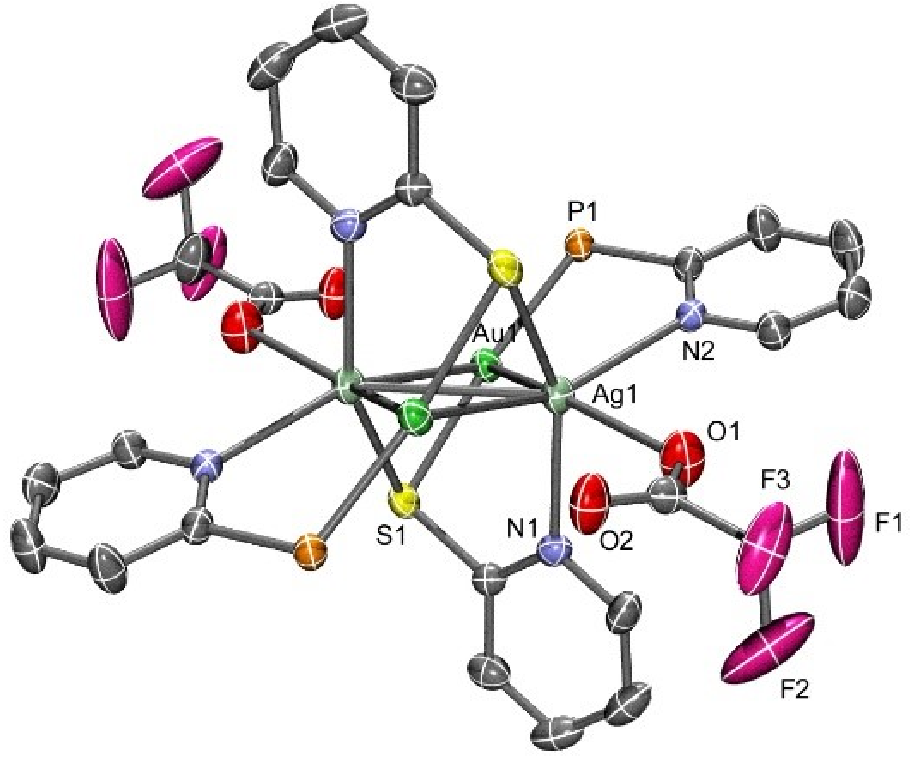
Poster Presentation : **INOR.P-9**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structures and Luminescent Properties of Heterometallic Au(I)-Ag(I) Complexes

Heehun Moon, Sung Kwang Lee, Daeyong Um, Young-A Lee*

Department of Chemistry, Chonbuk National University, Korea

A series of new Au(I)-Ag(I) heterometallic complexes, [AuAg(μ-Spy)(μ-PPh_2py)]X (X^- = BF_4^-, PF_6^-, ClO_4^-, $CF_3CO_2^-$, $CF_3SO_3^-$, NO_3^-), have been synthesized, and their optical properties have been studied in the solid state at room temperature and at 77 K. X-ray characterizations on the single crystals have provided the dimeric (**5**, X^- = $CF_3CO_2^-$; **6**, X^- = $CF_3SO_3^-$) or polymeric form (**7**, X^- = NO_3^-) of [AuAg(μ-Spy)(μ-PPh_2py)]X depending on the anion types. For **5** and **6**, the two of [AuAg(μ-Spy)(μ-PPh_2py)] moiety are bound via the transannular Ag-Ag interaction (3.03 – 3.07 Å) and bridging sulfur (Ag(1)-S(1), 2.50 – 2.54 Å: Au(1)′-S(1), 2.33 Å). Despite of the similar skeletal structure, **7** shows the infinite chains through the additional Au···Au interactions (2.8862(2) Å) and anion binding effects. At 77 K, Au(Spy)(PPh_2py) (**1**) complex shows emission band at 474 nm with long tail, while new Au(I)-Ag(I) complexes exhibit intense emission at 600 nm which is red-shifted on account of d^{10}-d^{10} interactions (aurophilic interactions, argentophilic interactions, and heterometallic Au(I)-Ag(I) interactions) and bridging sulfur ligands.


P1
Au1
Ag1
N2
O1
F3
F1
S1
N1
O2
F2

Poster Presentation : **INOR.P-10**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Dynamic Jahn-Teller effect in inorganic-organic hybrid perovskite $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA)

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The title compound is known as a layered inorganic-organic K_2NiF_4 type of general formula A_2MX_4 (A = organic cation, M = divalent metal, X = halogen). This layered inorganic-organic hybrid perovskite system has been investigated very long time, to elucidate the low-dimensional magnetic property and the effects of the interlayer distance variation on the magnetic behavior. According to the previous work, Cu-PEA has two structural phase transitions and one magnetic phase transition at 410K, 341K and at 13K, respectively. Based on the neutron single crystal study, the crystal structure at room temperature is totally ordered and due to Jahn-Teller effect, $CuCl_6$ octahedron in the Cu-PEA structure is strongly elongated. To predict the crystal structures at higher temperature, we made models using a crystal structure from neutron diffraction at room temperature. According to our model, the crystal structure should be totally disordered at higher temperature and if Jahn-Teller effect should further exist at higher temperature, $CuCl_6$ should show a distortion, which is a typical indication of an ordered character. But if the origin of Jahn-Teller effect is dynamic, the distortion of $CuCl_6$ octahedron can be cancelled out leading to non-distorted $CuCl_6$ octahedron. To check this effect in more detail, we conducted temperature dependent single crystal diffraction experiments at 300K, 380K and 430K using synchrotron beam at 2D beam line, Pohang Accelerator Laboratory (PAL), Korea. In this study, based on the crystal structures we will show Jahn-Teller effect in Cu-PEA is dynamic in origin.References[1] S. H. Park et al., (2012) Dalton Trans. 41, 1237.[2] A. O. Polyakov et al., (2012) Chem. Mater. 24, 133.[3[G. Heger, (1977) Habilitationsschrift, Karlsruhe.[4] G. Park et al., (2019) in preparation.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and electrochemical properties of CoFeP hollow nanostructure using ZIF template method

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New synthetic method was adopted to obtain CoFeP hollow nanostructures for electrocatalytic applications. The ZIF-67 nano-crystals are known as excellent structural templates to create uniform box structures with easy control of chemical composition and physical properties. The ZIF-67 of cube shape was prepared using CTAB, The hollow box structure of ZIF-67@CoFe-PBA was synthesized by acidic etching of ZIF-67 and addition of Fe (III) ion. Subsquent phosphidation of ZIF-67@CoFe-PBA resulted in hollow nanostructure of CoFeP. The products are characterized by XRD, XPS, SEM and TEM analyses. This hollow structures transition metal phosphide shows excellent electrocatalytic performances in water splitting process.

Poster Presentation : **INOR.P-12**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

N-doped microporous carbon derived from Zn-porphyrin MOF

Hyun-Chul Kim, Suk Bin Yoon, Suk Joong Lee[1], Sung-Jin Kim[2], Youngmee Kim[3], Seong Huh[*]

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[1]*Department of Chemistry, Korea University, Korea*
[2]*Department of Chemistry, Ewha Womans University, Korea*
[3]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

Metal-organic frameworks (MOFs) are valuable materials for various applications. A new Zn-porphyrin-MOF with a 3D hexagonal network structure was synthesized by solvothermal method. We introduced a simple self-templated synthetic route for N-doped MOF-derived carbon (MDC) using Zn-porphyrin-MOF. N-doped MDC was facilely prepared from direct carbonization of the porphyrin-MOF without additional carbon sources. The porosity was further controlled by conventional KOH activation. Both the BET surface area and total pore volume were enhanced with KOH activation. Development of microporosity during the activation process was confirmed by CO_2 sorption analysis. From these gas sorption analysis results, the KOH activation may induce positive effect on enhancement of electrochemical accessible surface area. Thus, we investigated electrochemical capacitive properties of the N-doped MDCs. At 0.2 A/g in 1 M H2SO4, the maximum values of specific capacitance and specific energy are 555.6 F/g and 40.4 Wh/kg, respectively. Also high rate capacitive performance with large specific power was shown in 6 M KOH up to 190 A/g. Furthermore, good recycling stabilities also can be seen up to 30,000 cycles.

Poster Presentation : **INOR.P-13**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Preparation of large-pore mesoporous silica nanospheres by a Ca ion-etching method using a cheaper Ca ion source

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A Ca ion-etching of the as-prepared mesoporous silica nanospheres (MSNs) containing ammonium-based organic template is a simple and efficient method for preparation of large-pore MSNs. In this facile process, the generation of new large mesopores through the partial collapse of several mesopores and the template removal through cation-exchange occurred simultaneously. However, the originally used Ca ion source, $Ca(NO_3)_2 \cdot 4H_2O$, is quite expensive for commercial applications. So we turned our attention to a Ca ion-etching of the as-prepared MSNs using a more cheaper source, $CaCl_2$. We found out that $CaCl_2$ could also behave as a good etchant. Template-free MSNs with large-pore could be obtained in high yield. We did protein sequestration experiments with the Ca ion-etched large-pore MSNs. The sequestration amounts using the $CaCl_2$-etched MSN were similar to the adsorption values for $Ca(NO_3)_2$-etched MSN. For bovine serum albumin (BSA, 66.5 kDa), the sequestration amount was 485 mg per 1 g of MSN. The adsorption value for smaller protein, ovalbumin (OVA, 42.7 kDa), was 584 mg per 1 g of MSN.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

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.

Poster Presentation : **INOR.P-15**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

In-situ synthesis of BiOClx/BiOBry/BiOIz nanofibers for visible-light photocatalytic investigation

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

In this work, BiOClx/BiOBry/BiOIz/PAN (x+y+z=1) composite nanofibers are prepared by electrospinning and sol-gel method. The photocatalytic degradation of trichloroethylene (TCE) over BiOClx/BiOBry/BiOIz/PAN nanofibers were investigated by gas chromatography method. Obtained from results, the optimum photocatalytic activity was achieved with BiOCl0.3/BiOBr0.3/BiOI0.4/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 BiOClx/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.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

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 photogeneration electron and holes between BiOCl and graphene oxide, and the better adsorption capacity of rhodamine B.

Poster Presentation : **INOR.P-17**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of bimetallic catalyst derived from Co/Ni containing Zeolitic-imidazolate Framework-67 (CoNi-ZIF) and Ni doped CoNi-ZIF-67 for oxygen reduction and evolution reactions

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[1]*Chemistry, Kunsan National University, Korea*
[2]*Department of Nano Chemistry, Gachon University Global Campus, Korea*

We have investigated the catalysts that have excellent performances for the oxygen evolution and reduction reactions in the zinc-air rechargeable batteries. Bimetallic CoNi embedded in the carbon nanotubes (CNT) were obtained by the calcination of CoNi-ZIF-67. We develop a general and high-yield strategy for the formation of CNT's from the CoNi-ZIF-67 at a temperature of 700°C by the calcination process. The formation of metallic Co/Ni embedded in the carbon nanotubes was investigated by the X-ray diffraction (XRD) and the graphitization was analyzed by the Raman Spectroscopy. The resulting CNT@CoNi-ZIF are highly porous with a high specific surface area of 242 m^2/g. After calcination, Ni deposition on the CNT's was performed. Moreover, surface area reduces to 168.7 m^2/g and structure is distorted due to deposition. The morphology and the presence of Ni on CNT's were proved by the TEM images. Furthermore, the porous Ni-doped CNT@CoNi-ZIF exhibited superior electrochemical performance as a cathode material for the Zn-air batteries. The cyclic test for charging & discharging was performed for 500 h revealing that the Ni deposited CNT's is a potential catalyst, showing splendid stability for the OER and ORR in the Zn-air batteries. **Keywords**: Bimetallic Catalyst, Oxygen Reduction Reactions, Oxygen Evolution Reactions, Zn-air battery, Carbon nanotubes

Poster Presentation : **INOR.P-18**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Coordinative Networking and Adaptive Guest Binding of Pillar[5]-*bis*-crowns

Mingyeong Shin, **Shim Sung Lee***

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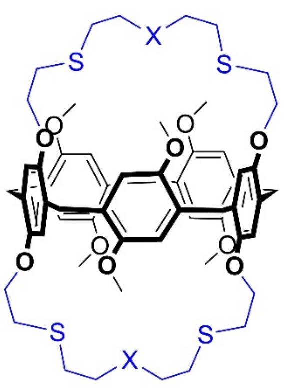
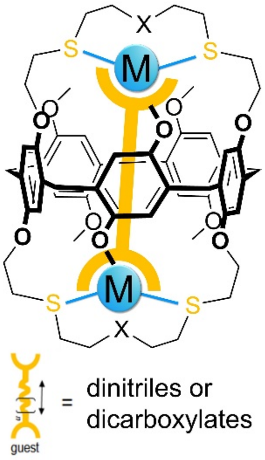
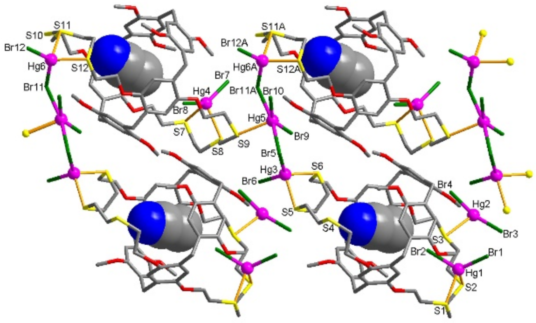
As extension of our previous works,[1-3] synthesis of pillar[5]-*bis*-crowns with different donor sets in the crown unit ($\mathbf{L^1}$: SNS and $\mathbf{L^2}$: SSS, *see* Fig. 1a) and their metallosupramolecules (**1**-**4**) are reported. First, assembly reactions of $\mathbf{L^1}$ with silver(I) salts (ClO_4^- and PF_6^-) afforded two isostructural disilver(I) complexes $[Ag_2(\mathbf{L^1})(ClO_4)_2]\cdot 2CH_2Cl_2$ (**1**) and $[Ag_2(\mathbf{L^1})(CH_3OH)_2](PF_6)_2\cdot 2CH_2Cl$ (**2**). In both complexes, the silver(I) center is four-coordinate, being bound to the SNS donors in the crown unit. As candidates for the bridging ligands for the linking of two silver(I) centers, dinitriles and dicarboxylates were employed to test the length-selective recognition concept (*see* Fig. 1b). When $\mathbf{L^2}$ was reacted with $HgCl_2$ (in CH_2Cl_2/CH_3OH) and $HgBr_2$ (in CH_2Cl_2/CH_3CN), we obtained a mononuclear complex $[HgCl_2(CH_2Cl_2@\mathbf{L^2})]$ (**3**) and a 1-D coordination polymer $[Hg_6Br_{12}(CH_3CN@\mathbf{L^2})_2]_n$ (**4**, *see* Fig. 1c), respectively, in which the mercury(II) atoms exist outside the cavity (exo-coordination). In **4**, two $CH_3CN@\mathbf{L^2}$ units are linked by a linear Hg_3Br_6 cluster via Hg-S bonds to form a C-type dimer and the adjacent dimers are further linked by other Hg-S bonds, giving rise a unique 1-D ribbon-type poly(dimer) chain structure.



X = NH ; **L**^{1}
X = S ; **L**^{2}





4, $[Hg_6Br_{12}(CH_3CN@\mathbf{L}^2)_2]_n$

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Formation of a Four-bladed Waterwheel-type Dicopper(II) Complex with Thiaoxa-macrocycle via an Adaptive Exo/exo-coordination Mode

Seulgi Kim, Shim Sung Lee*

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Two O_3S_2-macrocycles with different S⋯S distances ($\mathbf{L^1} < \mathbf{L^2}$) were employed as a strategy to isolate the adaptive products including a dicopper(II) complex via controlling exo-coordination modes. $\mathbf{L^1}$ gave a one-dimensional coordination polymer $[Cu_2(\mathbf{L^1})_2(NO_3)_4]_n$ (**1**) based on a convergent exo-coordination. Meanwhile, $\mathbf{L^2}$ resulted in the formation of a divergent exo-coordinated dicopper(II) complex $[Cu_2(\mathbf{L^2_{ox}})_4(\mu\text{-Cl})](NO_3)_4$ (**2**), in which four oxidized macrocycles ($\mathbf{L^2_{ox}}$) act as blades and Cu^{II}-(μ-Cl)-Cu^{II} entity as an axis shaft adopting a four-bladed waterwheel. The chloro-bridging ligand (μ-Cl) in **2** is derived from the dichloromethane solvent and stabilized by C-H⋯Cl^- H-bonding. The overall waterwheel structure is also stabilized by interligand C-H⋯O H-bonding to form a pseudo-cage. The present result demonstrates that a combination of the controlled exo-coordination and the induced species serve a consistent picture of the adaptive formation of a new type dicopper(II) complex with a highly organized structure.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Pairs of Dynamic-but-Tight Peanut Cage Isomers: Modulation/Isomerism via Anions, Anion Exchange, and Thermal Energy

SeongHyeon Park, SooMin Hyun[1], Ok-Sang Jung[2,*]

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A unique system on pairs of dynamic-but-tight peanut cage isomers, *endo*-Me_8-$[X_2@Pd_4L_8]X_6$ and *exo*-Me_4,*endo*-Me_4-$[X_2@Pd_4L_8]X_6$ (X^- = NO_3^-, BF_4^-, ClO_4^-; L = cyclohexyl(methyl)bis(3-pyridyl)silane) is set up. Self-assembly of $Pd(NO_3)_2$ with L produces *endo*-Me_8-$[(NO_3)_2@Pd_4L_8](NO_3)_6$ whereas the reaction of PdX_2 (X^- = ClO_4^- and BF_4^- obtained from anion exchange of $PdCl_2$ with AgX) with L gives rise to *exo*-Me_4,*endo*-Me_4-$[X_2@Pd_4L_8]X_6$. Anion exchange of endo-Me_8-$[(NO_3)_2@Pd_4L_8](NO_3)_6$ with X^- (X^- = ClO_4^- and BF_4^-) retains the isomeric skeleton *endo*-Me_8-$[X_2@Pd_4L_8]X_6$, and the anion exchange of *exo*-Me_4,*endo*-Me_4-$[(ClO_4)_2@Pd_4L_8](ClO_4)_6$ with NO_3^- maintain the isomeric cage, *exo*-Me_4,*endo*-Me_4-$[(NO_3)_2@Pd_4L_8](NO_3)_6$. Thus, three pair of peanut cage isomers have been efficiently constructed via both the direct self-assembly and the anion exchange. Another anion exchange of *endo*-Me_8-$[(NO_3)_2@Pd_4L_8](NO_3)_6$ with the bulky anion X^- (X^- = PF_6^- and $CF_3SO_3^-$) gives *endo*-Me_8-$[(NO_3)_2@Pd_4L_8]X_6$, in which only outside anions are exchanged without the change of nestled anions. The most important feature is that the isomers from the direct self-assembly are thermally more stable than those from the anion exchange, and thus each isomer from the anion exchange slowly returns to the corresponding isomer from the direct self-assembly in Me2SO above 80 oC without any decomposition. Their smooth anion exchangeability and concrete room temperature NMR spectra are evidence of unprecedented contradictory behavior on “dynamic-but-tight peanut cage isomers” in solution.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Hexafluorosilicate Anion: A Template for Coordination Cage

Jeyoung Lee

chemistry, Pusan National University, Korea

Jeyeong Lee, Sangwoo Lim, and Ok-Sang Jung**Department of Chemistry, Pusan National University, Busan 46241, Republic of Korea*The self-assembly of $Cu(BF_4)_2 \cdot H_2O$ with 1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane (L) at room temperature very slowly produce crystals consisting of the coordination cages, $[(SiF_6)@Cu_2L_4](BF_4)_2$. The reaction of CuX_2 ($X^- = BF_4^-$ and ClO_4^-) with L in the presence of $(NH_4)_2SiF_6$ fast gives rise to the cages $[(SiF_6)@Cu_2L_4](BF_4)_2$ and $[(SiF_6)@Cu_2L_4](SiF_6)$, respectively. Anion exchange of $[(SiF_6)@Cu_2L_4](BF_4)_2$ with NaX ($X^- = PF_6^-$ and NO_3^-) gives rises to a 2D structure of $[CuX_2L_2] \cdot H_2O$. The significant catalytic effects on catechol oxidation catalysis in dichloromethane have been observed in the order $[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH > [(SiF_6)@Cu_2L_4](SiF_6) \cdot > [Cu(PF_6)_2L_2] \cdot H_2O > Cu(BF_4)_2$.**Reference** [1] Lee, H.; Hwang, S. Y.; Malenahalli H. N.; Shim, Y.-B.; Jung, O.-S. *Cryst. Growth Des.* 2018, *18*, 1956-1960.

Poster Presentation : **INOR.P-22**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Reversible Structural Flexibility of Pd_6L_8 Cages via Recognition of Alkyl Sulfate Surfactants: The Alkyl Chains of Surfactants Predictions

Dongwon Kim, Soojin Lee, Ok-Sang Jung[1,*]

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

A new strategical study on a reversible molecular balloon of coordination cages was carried out. Self-assembly of palladium(II) nitrate with new tridentate 1,3,5-tris(4-nicotinamide-phenoxy)benzene (L) produces $[Pd_6L_8]^{12+}$ cages with an inner cavity of 19 × 21 × 25 Å^3. The successive anion exchange of nitrate with alkyl sulfates ($ROSO_3^-$, R = ethyl-, octyl-, decyl-, dodecyl-, and tetradecyl-) produces a host-guest interaction between the cage and alkyl sulfates, inducing the contraction of coordination cages with an inner cavity of 13 × 13 × 13 Å^3. The alkyl sulfates specifically act as a molecular glue via hydrogen bonds between the oxygen of the sulfate and the hydrogen of the amide moiety, thereby enabling the coordination cage to recognize the length of the alkyl sulfate surfactants. The contact angles of a drop of liquid on the surface of find-ground crystalline solids are strongly dependent on the alkyl chain length of the included alkyl sulfates.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Flexible Molecular Double Cages as Ruler for Various Anions: Construction and Anion Exchange of $[X_2Pd_3L_4]^{4+}$ Double Cages

Ahreum Kim, Hyejin Oh, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

The stepwise reactions of Pd(II) with new tridentate donor (bis(pyridin-3-ylpropyl) pyridine-3,5-dicarboxylate) efficiently construct a double cage system, $[(X)_2Pd_3L_4](X)_4$ ($X^- = NO_3^-$, BF_4^-, ClO_4^-, PF_6^-). A variety of counteranions were employed to investigate the different behavior of the double cages. The choice of the counter anion did not influence the formation of mononuclear complexes whereas the counter anion displayed a template role for the formation of trinuclear double cages. When anion exchange via NaX or NH_4X was accomplished, the skeletal structure of double cage varies flexibly with the magnitude of the anion inside the cage.

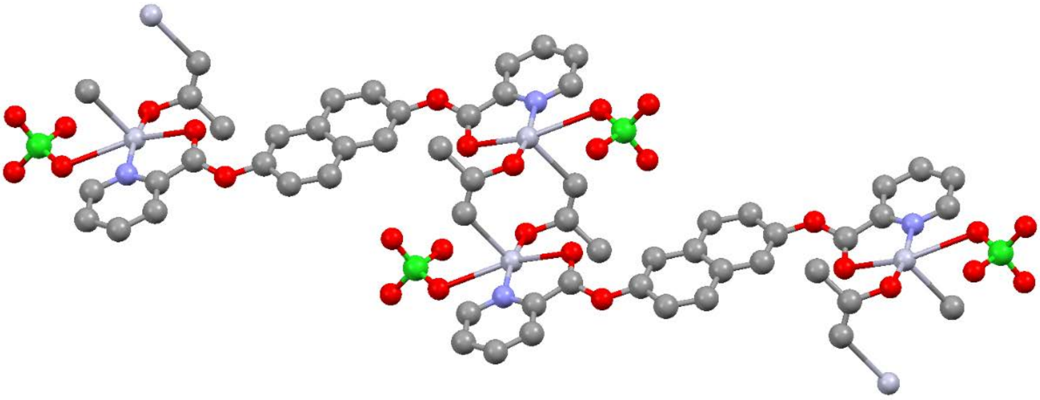
Poster Presentation : **INOR.P-24**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Formation and Structures of Metal-Organic Frameworks Including Enolate

EunSoo Yi, Junhee Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of Hg(ClO$_4$)$_2$ with L(L=naphthalene-2,6-diyldipicolinate, naphthalene-2,6-diyldiisonicotinate) form metal-organic frameworks in a mixture of dichloromethane and acetone. Acetone molecules from solvent turn into enolate moiety. In the crystal structures, two enolate moiety bridged two Hg(II) ion. The alkylation of enolate molecules with haloalkane is in progress.



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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Thermally Activated Delayed Fluorescent Properties of *Ortho*-Donor-Appended Oxaborin Compounds

Juhee Kim, Hanif Mubarok, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

Highly efficient thermally activated delayed fluorescent (TADF) compounds were prepared based on *ortho*-donor-appended oxaborin structures (BuCz*o*OB, DMAC*o*OB, PXZ*o*OB). For comparison, dimesitylboron acceptor containing compound was also prepared (DMAC*o*B). X-ray crystal structure of DMAC*o*OB showed that DMAC and oxaborin rings are perpendicular to each other, as judged by the dihedral angles of 90.0°. All of compounds were highly emissive in oxygen-free toluene and in particular, DMAC*o*OB exhibited 100% PLQY. PL spectra showed different emission color ranging from blue to orange depending on the donor group. All compounds except for BuCz*o*OB also showed strong TADF character. The details of synthesis, characterization, and comparison of photophysical properties will be discussed.

Poster Presentation : **INOR.P-26**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

A diamine-grafted metal-organic framework with excellent regeneration energy efficiency and CO_2 capture properties

Minjung Kang, Dong Won Kang, Jong Hyeak Choe, Hyojin Kim, Jeoung Ryul Park, Jinkyoung Park, Daewon Kim, Yun Seok Chae[1], Chang Seop Hong[*]

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

Recently, amine-grafted metal-organic frameworks (MOFs) have been reported to show excellent CO_2/N_2 selectivities and adsorption characteristics. Its CO_2 adsorption and desorption behaviors are controllable by altering the amine structure. We synthesized Mn-based MOFs and functionalized with various diamines to enhance the CO_2 adsorption ability and regeneration energy efficiency. The captured CO_2 in the MOFs can be desorbed at low temperatures, which leads to minimization of the total regeneration energy. These Mn-based MOFs were characterized by PXRD, infrared spectroscopy, and gas sorption. Additionally, CO_2 adsorption capacity was evaluated by thermogravimetric analysis (CO_2 15% / N_2 85%). Detailed synthetic scheme and specific properties will be presented in the poster.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Adsorption of carbon dioxide from indoor air by diamine-functionalized metal-organic frameworks

Jeoung ryul Park, Saemi Kim[1], Jee Yeon Kim[1], Dong Won Kang, Minjung Kang, Jong Hyeak Choe, Daewon Kim, Jinkyoung Park, Yun Seok Chae[2], Chang Seop Hong[*]

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High concentration of carbon dioxide in indoor air has various adverse effects on the human body. Normally, the concentration of carbon dioxide in the atmosphere is 400 ppm, but it can increase above the recommended CO_2 level of 1000 ppm in a room. We have functionalized metal-organic frameworks (MOFs) with several diamines to adsorb carbon dioxide in confined spaces. In particular, these compounds can desorb carbon dioxide at relatively low temperature. Diamine-functionalized MOFs were characterized by infrared spectroscopy, thermogravimetric analysis, and gas sorption. Detailed properties and synthetic scheme will be given on the poster.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Postmodification of amine-grafted Mg_2(dobpdc) composite for carbon dioxide capture in humid conditions

Jong Hyeak Choe, Chang Seop Hong[*], Hyojin Kim[1], Minjung Kang, Dong Won Kang, Jeoung Ryul Park[1], Daewon Kim[1], Yun Seok Chae[2], Jinkyoung Park[1]

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

We have synthesized Mg_2(dobpdc) composite for carbon dioxide capture. Using post-synthetic modification method, *N*-ethylethylenediamine functionalized Mg_2(dobpdc) composite was prepared and it has high CO_2 adsorption capacity. To improve water stability of this composite, hydrophobic silane was added in Mg_2(dobpdc) composite. The crystallinity of the Mg_2(dobpdc) composite was maintained under humid conditions. This compound was characterized *via* X-ray diffraction, infrared spectroscopy and thermogravimetric analysis. Detailed specific properties will be presented in the poster.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis of Bimetallic Metal-Organic Framework from a One-Dimensional Zn-based Precursor

Hyojin Kim, Chang Seop Hong[1,*], Dong Won Kang[1], Minjung Kang[1], Jong Hyeak Choe[1], Jeoung Ryul Park, Daewon Kim, Jinkyoung Park, Yun Seok Chae[2]

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

Mixed metal-organic frameworks (MOFs) have attracted much attention because of enhanced functionalities, such as gas adsorption and catalysis. Herein, we synthesized a bimetallic Mg/Zn(dobpdc) (H_4dobpdc= 4,4'-Dihydroxy-(1,1'-biphenyl)-3,3'-dicarboxylic acid) constructed from a one-dimensional Zn precursor. In particular, the bimetallic Mg/Zn(dobpdc) has remarkably ordered 1:1 heterogeneity of Mg and Zn in the framework structure, which would not be obtained by the conventional reaction of the corresponding metal salts. The bimetallic Mg/Zn(dobpdc) was characterized by powder x-ray diffraction, infrared spectroscopy, TEM-EDS, and ICP-AES. Detailed synthetic scheme and characterization will be presented in the poster.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Ortho-Donor-Acceptor TADF Compounds with Different Triarylboron Acceptors

Hanif Mubarok, Juhee Kim, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

Triarylboron acceptor in the donor-acceptor compounds plays a crucial role in attaining strong thermally activated delayed fluorescence (TADF) properties. To investigate the effect of boron acceptor on the TADF properties, we prepared a series of *ortho*-D-A compounds based on 9,9-diphenyl-9,10-dihydroacridine (DPAC) as a fixed donor and different triarylboron moieties as an acceptor. Planarized cyclic triarylborons, such as boraanthracene (DPAC*o*DB) and oxaborin (DPAC*o*OB), as well as dimesitylboron (DPAC*o*B) were employed as electron-accepting units. All compounds showed high photoluminescence quantum yield (PLQY = 91-99%) in solution and strong TADF character. The details of synthesis, characterization, and comparison of photophysical properties will be discussed.

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

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and characterization of Cu(II) complexes bearing (+)-Camphor derivative of (E or R , S)-1-(2-Pyridyl)ethylamine

Juhyun Cho, Jong Hwa Jeong*

Department of Chemistry, Kyungpook National University, Korea

The discovery and development of novel chiral ligands are of significant importance in asymmetric catalysts. So we synthesized α-methyl-N-[(1R, 4R)-1,7,7-trimethylbicy-clo-[2.2.1]hept-2-ylidene]-(E)-1-(2-pyridyl)ethylamine (PIC) ligand and separated them into RRS, RRR form. This ligands have led to C1-symmetric ligand with two differentiated N (sp^2) atoms and provide highly sterically differentiated surroundings for both equatorial coordination sites of the Cu(II). The X-ray crystal structure of Cu(II) complex containing PIC was determined. In case of diastereomer mixture PIC were (1R,4R)(S) and (1R,4R)(R)-coordination Cu(II) complexes were co crystallized. The geometry around the Cu(II) centre for (PIC)$CuCl_2$ were distorted squere-planner for all cases of RRR and RRS as well.

Poster Presentation : **INOR.P-32**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Electrophoretic deposition of Iron Oxide thin films as anode electrode materials for pseudocapacitor

Yo Seob Won, Duk-Young Jung[1,*]

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

Iron oxide (α-Fe_2O_3) has been investigated intensively as a promising anode material in supercapacitor application due to their advantages such as high theoretical capacity, non-toxicity, low cost, natural abundance, high resistance to corrosion. This work reports the synthesis, characterization, and electrochemical properties of amorphous hematite thin films. These nanostructures were characterized using powder X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM). The thickness of the deposited hematite thin films was measured from the Alpha-step profiler analysis. We used the electrophoretic deposition technique to prepare positively charged iron oxide layer in formamide on the Ni metal substrates. Scanning electron microscopy results reveal that the hematite thin films have well covered surface of Ni metal substrate. The electrochemical performances were evaluated by using the three electrodes cell system within aqueous KOH electrolyte showing a high capacitance around 800 F/g.

Poster Presentation : **INOR.P-33**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Surface modification of a metal-organic framework Cr-MIL-101 with amine and carboxylic acid for attachment of alcohols through hydrogen bonds

Jongbum Oh, Jiwon Kim, You Jin Oh[1], Jaheon Kim[1,*]

Soongsil University, Korea
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Cr-MIL-101 formulated as [Cr3O(BDC)3(H2O)2(OH)] (BDC = benzene-1,4-dicarboxylate) was functionalized with –NH2, -COOH, or –NH2/COOH to give Cr-MIL-101-NH2 (1), Cr-MIL-101-pCOOH (2), and Cr-MIL-101-NH2/COOH (3), respectively. These MOFs have hydrophilic surfaces and can form hydrogen bonds with alcohol molecules. As expected, methanol adsorption/desorption isotherms at room temperature indicated that (3) has the largest affinity to methanol molecules. Due to this property, (3) could extract alcohol molecules in organic solvent such as methylene chloride. By taking advantage of this alcohol affinity, various alcohols and diol isomers could be easily introduced to the surface of (3) to produce alcohol-adsorbed MOFs. Gas adsorption experiments indicated that the hydrogen-bonded alcohols can affect the affinity of the MOFs to CH4 gas at room temperature. These results show that the porosity of MOFs can be adjusted by attaching surface-modifiers through non-covalent bond in a reversible way.

Poster Presentation : **INOR.P-34**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Syntheses of isoreticular metal-organic frameworks functionalized with alkoxy groups for enhanced methane storage at room temperature and under high pressure

Jeonhyeong Kwon, Jisu Lee[1], Kyungkyou Noh[2], Jaheon Kim[3,*]

Chemistry, Soongsil University, Korea
[1]*Soongsil University, Korea*
[2]*Department of ICMC convergence technology, Soongsil University, Korea*
[3]*Department of Chemistry, Soongsil University, Korea*

Methane, which has a relatively large heat of combustion, can be used for a clean fuel in vehicles. For efficient storage of methane at room temperature, porous solids such as MOFs have been extensively investigated to meet a volume storage capacity of 263 cm3/cm3 at room temperature and under 65 bar set by DOE. However, neglecting a volume loss in materials packing, the maximum working capacity of the best MOF to date is only 197 cm3/cm3 between 5 and 65 bar. Thus, to achieve a desirable storage capacity, it is necessary to find out key parameters that can correlate storage capacity with the structures, interacting sites, and porosity of MOFs. For this goal, we synthesized a series of IRMOFs by solvothermal reactions between Zn ion and linear ligand such as H2BDC-M (2,5-dimethoxyterephthalic acid), H2BDC-E (2,5-ethoxyterephthalic acid), H2BDC-P (2,5-dipropoxyterephthalic acid), and their mixtures, respectively. XRD analyses indicated that these MOFs have the same pcu-topology as MOF-5. The methane adsorption behaviors of these MOFs measured respectively at room temperature and under 1 bar, and 70 bar could be correlated to their specific surface areas, pore volumes, and functional groups. Based on these results, we propose empirical parameters for an optimized methane storage capacity of the IRMOFs.

Poster Presentation : **INOR.P-35**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Hydrothermal synthesis, structures, and characterization of new quaternary iodates

Geonju Park, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

New quaternary iodate crystals have been successfully synthesized by a hydrothermal method. It has been well known that d^0 transition metal cations in octahedral coordination environment are a good noncentrosymmetric (NCS) chromophore revealing nonlinear optical properties. However, compounds containing transition metal cations tend to exhibit small band gaps due to d orbital. In order to synthesize materials showing large band gaps, main group metals were introduced. Single crystal X-ray diffraction shows that the reported materials crystallize in the centrosymmetric space groups, P-1 and $P2_1/c$ and exhibit unidimensional chain structures. Synthesis, structures, and spectroscopic characterizations are presented.

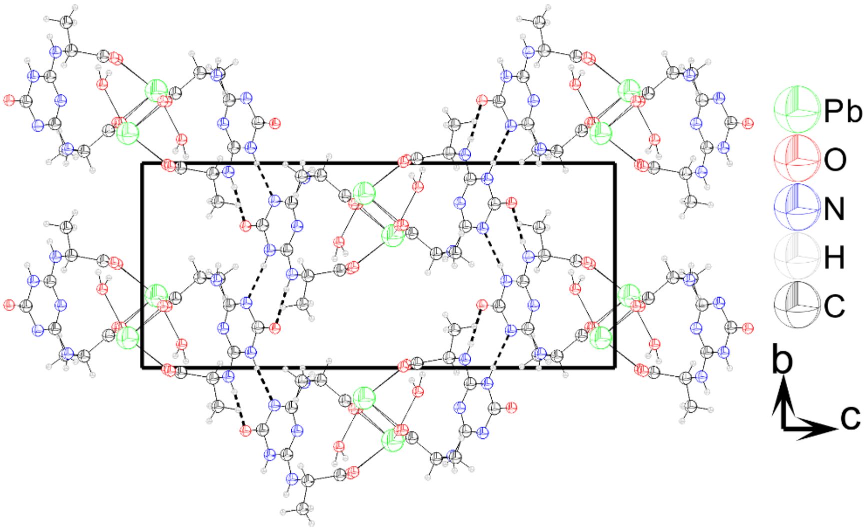
Poster Presentation : **INOR.P-36**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

A New Pb-based Non-centrosymmetric Coordination Polymer with a Chiral Organic Ligand

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

A new lead-based coordination polymer (**1**) was synthesized through a hydrothermal reaction at 100 ℃. The introduced organic linker was initially prepared by a nucleophilic aromatic substitution reaction (S_NAr). The structure of compound **1** was determined by single crystal X-ray diffraction (SC-XRD). Compound **1** crystallized in the orthorhombic non-centrosymmetric space group, $P2_12_12_1$ possibly because of the chiral organic ligand. The Pb^{2+} cation reveals distortive PbO_7 polyhedra with oxygen atoms from carboxylate and water. The carboxylate groups in the linkers contain two kinds of coordination modes, i.e., a chelating mode and a chelating/bridging mode. Compound **1** reveals an infinite chain structure, in which the chains are bridged by quadruple hydrogen bonds with organic ligands (N-H···O 2.094 Å, N-H···N 2.033 Å). Considering the hydrogen bonding interactions, pores with the size of ca. 7 Å x 10 Å are formed from the structure.


Pb
O
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Poster Presentation : **INOR.P-37**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Competitive and Selective Formation between 2D and 3D Metal-Organic Frameworks

Sojin Oh, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The structural dimension of metal–organic frameworks (MOFs) is of great importance in determining their properties and thus applications. Especially, two-dimensional (2D) layered MOFs are of considerable interest due to their valuable applications. Distinctive structural features of 2D materials, such as large number of open active sites and high surface areas, are known to facilitate their utilizations. Herein, we report a methodology for the selective synthesis of a 2D MOF in the presence of the competitive formation of a three-dimensional (3D) MOF. The ratio between metal ions and organic building blocks, used during the reaction, is found to be important for the selective formation of 2D MOF, and is associated with its chemical composition. Furthermore, the well-defined micro-sized 2D MOF particles with a narrow size distribution are synthesized in the presence of an ultrasonic dispersion. Moreover, the laminated 2D MOF layers are directly synthesized via a modified bottom-up lamination method, a combination of chemical and physical stimuli, in the presence of surfactant and ultrasonication.

Poster Presentation : **INOR.P-38**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Bimetallic Conductive Two-Dimensional Metal-Organic Framework and Its Enhanced Electrochemical Oxygen Reduction Activity

Jian Yeo, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The development of new electrocatalysts for electrochemical oxygen reduction to substitute the expensive and rare platinum-based catalysts is a central issue in energy storage and conversion. In this context, conductive and porous metal-organic frameworks (MOFs) are considered promising materials for the oxygen reduction reaction (ORR) due to not only their high surface area and well-developed pore but also versatile structural features and chemical compositions. Herein, we report the construction of bimetallic conductive two-dimensional MOFs (named CoxNiy-CATs) for use as catalysts in the ORR. The ratio of the two metal ions in the bimetallic CoxNiy-CATs is rationally controlled to determine the best composition for efficient performance in the ORR. Indeed, bimetallic MOFs display the enhanced ORR activities compared to their monometallic counterparts (Co-CAT or Ni-CAT). Bimetallic CoxNiy-CATs retain an advantageous characteristic of Co-CAT in relation to its high diffusion-limiting current density, as well as a key advantage of Ni-CAT in relation to its high onset potential. Furthermore, the ORR-active bimetallic CoxNiy-CAT with an excellent ORR activity is prepared at a large scale via a convenient method using a ball-mill reactor.

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

Inorganic Chemistry

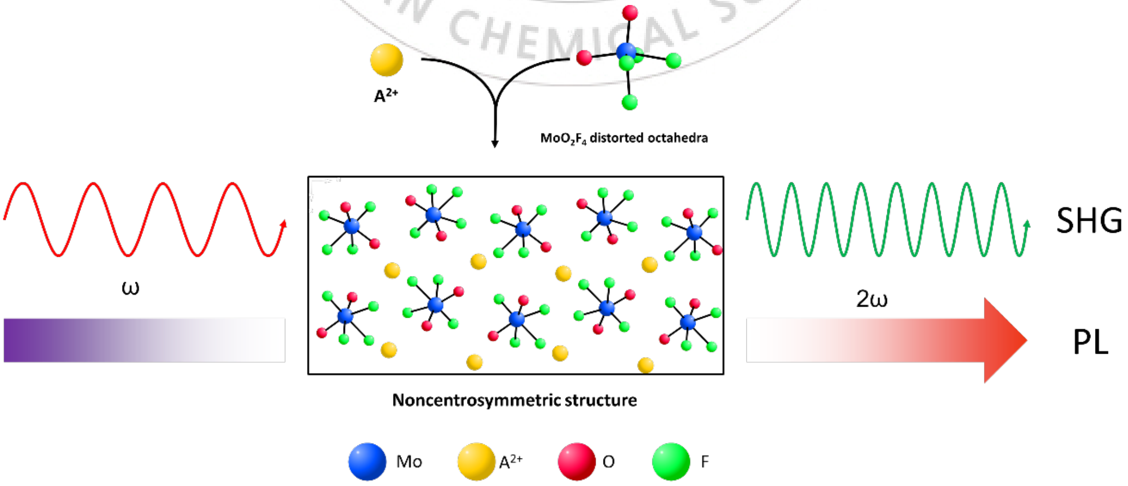
Exhibition Hall 1, THU 11:00~12:30

Nonlinear optical properties of a series of new noncentrosymmetric molybdenum oxyfluorides

Hongil Jo, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

We have synthesized a series of new noncentrosymmetric molybdenum oxyfluoride compounds through hydrothermal reactions. The structures of the reported materials are composed of $MoO_2F_4^{2-}$ octahedra and charge balancing cations. Mo^{6+} ions have two short bonds with oxide ligands in *cis*-position, and two intermediate and two long bonds with fluorides. All $MoO_2F_4^{2-}$ octahedra reveal local C2 distortions. Because the MoO_2F_4 units are not aligned in anti-parallel manner, the compounds crystallize in the polar space group, $Pca2_1$. Second harmonic generation (SHG) measurements indicate that the reported materials have similar SHG efficiencies to that of α-SiO_2. Furthermore, the title compounds exhibit photoluminescence properties attributed to the ligand to metal charge transfer in $MoO_2F_4^{2-}$. Detailed spectroscopic and thermal analyses are also presented.



Poster Presentation : **INOR.P-40**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Superexchange Effect on Thermopower: Thermoelectric Characteristics of Oligo(Ethylene Glycol) in Large-Area Molecular Junctions

Nayoung Cho, Seohyun Kang, Jiwoong Jang, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Understanding the charge transport phenomena across organic and organometallic molecules is important for a wide range of research fields ranging from materials science to molecular biology and nanoelectronics. Charges usually traverse through organic molecules in an off-resonant tunneling regime for many cases. Hence, charge transport and thermovoltage creation across single molecules or ensembles of molecules are usually described by a transmission function in molecular electronics and thermoelectrics. Superexchange tunneling has been often studied in molecular biology, yet little is known about how it affects thermopower of molecules. We investigated charge transport across thiol-terminated oligomers of ethylene glycol ($HS(CH_2CH_2O)_nCH_3$; $HS(EG)_nCH_3$, n = 1 - 5) using a large-area junction having the structure $Au^{TS}/SAM//Ga_2O_3/EGaIn$, where Au^{TS} is a template-stripped gold surface, SAM is the self-assembled monolayer, and $Ga_2O_3/EGaIn$ is the eutectic gallium-indium covered with a native gallium oxide layer. We measured tunneling conductivity, thermovoltage, and Seebeck coefficient on the identical junction platform and explored the length dependence of these. In particular, we compared thermopower between the ethylene glycol-based SAMs and the corresponding alkyl SAMs ($HS(CH_2)_nCH_3$, n = 3, 6, 9, 12, 15) to examine the effect of superexchange tunneling on thermopower.

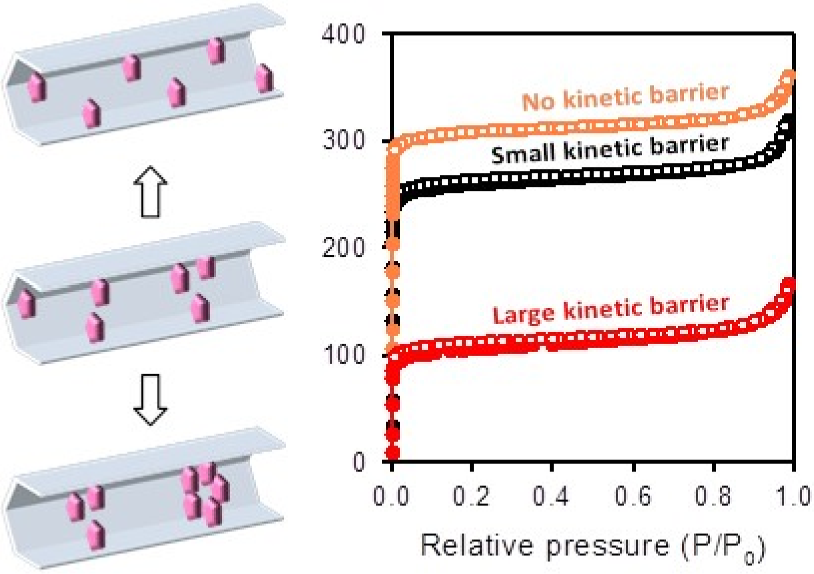
Poster Presentation : **INOR.P-41**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecule Positioning in 1-D Channel of MOF-74 for Efficient Hydrogen Isotope Separation

Junsu Ha, Jin Yeong Kim, Hoi Ri Moon*

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

Metal-Organic frameworks (MOFs) with highly porous structure and unprecedented tunability have attracted a lot of attention in addressing various challenging separation processes. The separation efficiency of MOF-based system depends on the host-guest interaction, thus, optimizing the pore environment suitable for a target molecule is a key for improving separation performance, selectivity and capacity. Several studies have been conducted to modify the pore environment, such as introducing various molecules via post-synthetic modification. So far, however, there is an inevitable problem that a large amount of molecule introduced to obtain an optimum pore structure occupy pores and lower the adsorption capacity. Therefore, it is important to develop a new strategy to obtain optimal pore environment with high selectivity while minimizing the loss of separation capacity. Herein, we present variation in the distribution of incorporated molecule into 1-D channel MOF which having open metal sites, induced by various inclusion methods or additional treatment after the molecule inclusion via post-synthetic modification. Despite the same amount of incorporated molecule, adsorption amounts and hysteresis loop in both N_2 and H_2 sorption isotherms were remarkably varied after the additional treatments (heating, pressure), meaning the variation of pore environment. In our expectation, this positioning strategy can be a key for controlling both separation and storage performance and can be applied to synthesize separating material having high selectivity without loss of adsorption capacity, especially for H_2/D_2 separation.


No kinetic barrier
Small kinetic barrier
Large kinetic barrier
400
300
200
100
0
0.0
0.2
0.4
0.6
0.8
1.0
Relative pressure (P/P0)

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **INOR.P-42**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

In situ High Temperature XRD study of Bismuth Titanate.

Dongwoo Lee

Nuclear Chemistry Research Team, Korea Atomic Energy Research Institute, Korea

Noncentrosymmetric(NCS) materials are of topical and technological interest, because of their second harmonic generation (SHG), piezoelectric, ferroelectric, and pyroelectric properties.With oxide materials, the asymmetric coordination environments are normally observed in two families of metal cations, octahedrally coordinated high valent d0cations (Ti^{4+}, Nb^{5+}, Mo^{6+}, etc.) and cations containing nonbonded electron pairs (Sb^{3+}, Bi^{3+}, Se^{4+}, Te^{4+}, etc.). With both families of cations, the primary distortive cause could be attributable to electronic second-order Jahn-Teller (SOJT) effects.The Bi^{3+} cation has been a very important node in the building of interesting functional materials, since Bi3+ can exhibit variable coordination numbers, framework flexibilities, and diverse structural characteristics.Also, Bi^{3+} cation inherently possesses an asymmetric structural geometry attributed to the lone pair. The Ti^{4+} cation has been well known that materials containing lone pair cations tend to exhibit local asymmetric coordination environments.Bismuth titanate materials have been continuously attracted by materials scientists owing to their fascinating characteristics such as magnetic, superconductive,dielectric, thermoelectric, electrocatalytic, ferroelectric, and optical properties.In this study, various structural types of bismuth titanates have been observed using in-situ XRD.

Poster Presentation : **INOR.P-43**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

SuFEx-based Post-synthetic Modification of Metal-organic Frameworks

<u>Seungjae Park</u>, Eunsung Lee*

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

Metal-organic frameworks (MOFs) are representative robust and porous crystalline materials consisting of metals and organic linkers. In the past few decades, numerous metal-organic frameworks (MOFs) and their synthetic methods have been reported to develop their interesting applications. Among various methods, post-synthetic modification (PSM) strategies have been mainly utilized to introduce novel properties in the MOFs. The first option to introduce the property is to modify the organic linkers. Recently, a new type of PSM strategy utilizing sulfur(VI) fluoride exchange (SuFEx) was reported. With this method, several functional groups were successfully substituted with high yields. Here we report two novel MOFs with sulfonyl fluoride that is possible for PSM via SuFEx. They are successfully characterized by SXRD, PXRD, and gas sorption. Currently, the applications using these materials are currently in development.

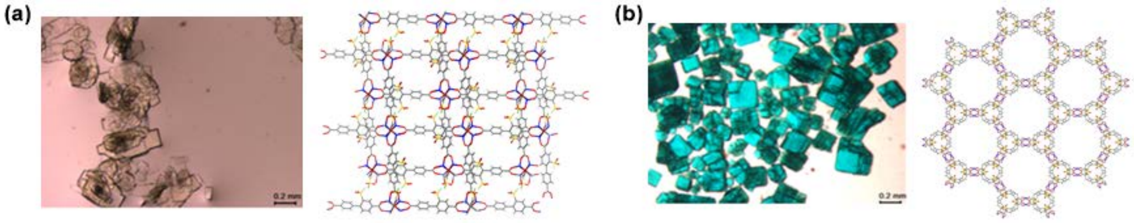


Figure 1. The crystals and frameworks of (a) Zn-3D framework and (b) Cu-3D framework.

Poster Presentation : **INOR.P-44**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Properties of water-soluble Ruthenium Nitrosyl Complexes with Schiff base ligand

Minyeong 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. Previously, we introduced ruthenium nitrosyl complexes with hydroxyl group on the positions of ortho, meta and para of the salophen ligand. This research aims at developing ruthenium nitrosyl complexes which dissolve in water. Here, we show the NO-releasing properties of the complexes monitored by IR, UV-VIS, EPR and X-ray crystallography. The complex Ru(NO)(salophen)Cl was found to release the nitrosyl ligand, upon exposure to UV/Vis light, and it was confirmed that the solvent bonded in place. Also EPR data can be interpreted as that the diamagnetic [Ru-NO]6 electronic state of the complexes change to paramagnetic properties Ru(Ⅲ) (d5, S=1/2) upon losing NO.

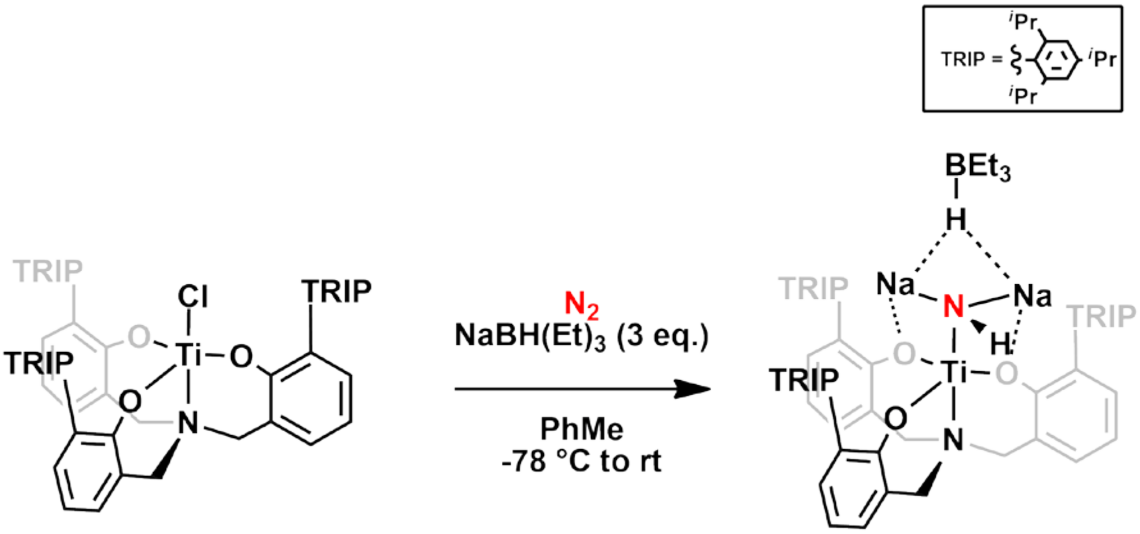
Poster Presentation : **INOR.P-45**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

A Mononuclear Titanium-imide Complex Derived from Dinitrogen Splitting

Dae Young Bae, Eunsung Lee*

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

Activation and cleavage of dinitrogen is an important and challenging subject because this most earth abundant gas, which has a strong bond (BDE = 225 kcal/mol), can be converted into value added compounds such as a N1 source. In nature, nitrogenase transforms nitrogen to ammonia under ambient conditions, whereas the Haber-Bosch process converts it to ammonia under harsh conditions for mass production. Although there has been intensive investigation on transformation of dinitrogen to value-added compounds in a homogenous system under mild conditions for the last decades, there is still a huge interest in cleaving and functionalizing nitrogen molecule with a well-defined system to accumulate all the N_2 activation information for developing a better system. Here, we present a mononuclear titanium-imide complex with sodium triethylborohydride. This complex results from a complete cleavage of dinitrogen by a sterically encumbered titanium aminotriphenolate complex. Most of reported dinitrogen cleaved complexes are occurring with a dinuclear or multinuclear system, but our N_2 cleaved complex shows mononuclearity. We assumed that it is mainly because of sterically encumbered ligand. We also confirm that the imide ligand, derived from N_2 splitting, is able to afford ammonium cation when proton sources are treated. Currently, we are investigating its reactivity and mechanisms for the formation of the complex.



Ti-Cl

Ti-N

18% as crystal

124th General Meeting of the Korean Chemical Society
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Poster Presentation : **INOR.P-46**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of Benzoxazole-Functionalized Metal-Organic Frameworks

Dasom Kim, Hyeon Bin Ha[1], Min Kim[1,*]

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

Metal-organic frameworks are organic-inorganic hybrid materials, which are consisting of multitopic coordinating ligands and metal clusters (or ions). The multitopic ligands could have additional functional groups in their C-H bond sites, and various functional groups such as amino, nitro, halo, hydroxy, and additional aromatic rings have been successfully incorporated into MOFs through ligand functionalization. The chemical handles in MOFs could be converted to other functionalities in the solid-state manner, which called post-synthetic modification (PSM). Traditional organic transformations such as acylation from amino group, cyanation from bromo group have been accomplished through PSM strategy.[1]Recently, we have successfully prepared several bifunctional MOFs with two chemical handles such as NH2, NO2, OMe, and Cl functionalities.[2] Besides the original studies were focused on the structural flexibility changes of MOFs with regioisomeric ligands, herein, PSM with two reactive chemical handles has been performed to obtain benzoxaole moiety. The selective PSM were performed with positional changes of functional groups. The detail synthetic procedures along with characterization of ligands and MOFs will be discussed.References1 Kim, M.; Cohen, S. M. *CrystEngComm*, **2012**, *14*, 4096.2 Ha, H.; Hahm, H.; Jwa, D. G.; Yoo, K.; Park, M. H.; Yoon, M.; Kim, Y.; Kim, M. *CrystEngComm*, **2017**, *19*, 5361.

Poster Presentation : **INOR.P-47**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Carborane-Functionalized Metal-Organic Frameworks for Photophysical Properties

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

The general icosahedral carborane ($C_2B_{10}H_{12}$) is cage type molecule, and it shows high thermal stability and chemical resistance, unique geometry and photochemical properties. Carboranes are utilized in a variety application such as heat-resistant polymers, catalysis, recovery of heavy metals from solution, and medical applications. In addition, the photochemical and electrochemical applications have been widely studied since the carborane cage has electron-deficient properties and affects the π-conjugation emission characteristics. Metal-Organic Frameworks (MOFs) are three-dimensional porous crystalline materials, which are consisted of metal clusters and multitopic organic ligands. Since MOFs are generally synthesized from solvothermal condition and shows structural rigidity, the introduction of carboranes into MOFs have been attempted by several research teams. Particularly, the benzene rings on MOF's ligand were replaced with carborane cages. In this presentation, we will discuss our recent results about the synthesis of carborane-functionalized MOFs along with their unique photophysical properties. The photoluminescence spectra for carborane-functionalized MOFs will be compared and presented.

Poster Presentation : **INOR.P-48**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Flexibility Controls of Metal-Organic Frameworks within Regioisomerisms

Dopil Kim, Hyeon Bin Ha, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-Organic Frameworks (MOFs) are coordination materials, which are consisting of metal clusters (or ions) and multitopic organic ligands. MOFs generally have three-dimensional frameworks with permanent porosity, and sometimes they have flexible frameworks. The flexibility of MOFs (i.e., structural changes of MOF frameworks) is induced by external stimuli such as pressure, guest molecular contact, solvent, etc. Recently, it was revealed that the position of organic functional groups and related electronic density of ligands are directly correlated with the flexibility of MOFs. Among the various combination of two functionalities, only NH_2-Cl, NH_2-Br, NH_2-OMe, OMe-OMe combinations showed the flexibility changes by the 2,3- or 2,5- position controls of functional groups in ligands. (i.e., ortho- and para regioisomeric of functional group).[1-3] In this presentation, we will discuss our recent studies for metal cation effect of flexibility in DMOFs. DMOF structure with three different metals (Co, Cu and Zn) were obtained with regioisomeric ligands, and studied for flexibility changes. These findings are also supported by computational approaches. In addition, the mixed ligand strategies have been also applied to regioisomerism of MOFs with 2,3- and 2,5- OMe-OMe ligands. The preparation of ligands along with MOF syntheses, and their structural changes to evacuation will be presented within regioisomeric manners.References1 Kim, M.; Boissonault, J. A.; Dau, P. V; Cohen, S. M. *Angew. Chem. Int. Ed.* **2011**, *50*, 12193.2 Hahm, H.; Yoo, K.; Ha, H.; Kim, M. *Inorg. Chem*. **2016**, *55*, 7576.3 Ha, H.; Hahm, H.; Jwa, D. G.; Yoo, K.; Park, M. H.; Yoon, M.; Kim, Y.; Kim, M. *CrystEngComm*, **2017**, *19*, 5361.

Poster Presentation : **INOR.P-49**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Unravelling a unified mechanistic principle of the tubular shape evolution of microporous organic polymer using ionic building blocks.

Chang Wan Kang, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

The functional performance of microporous organic polymers (MOPs) is dependent on their morphological structures. MOPs can be prepared by various coupling reactions of organic building blocks. Among the coupling reactions, the Sonogashira coupling has been proven to be a very efficient method.In the synthesis of MOP materials based on the Sonogashira coupling, the unexpected formation of tubular MOPs has been reported. However, the mechanistic understanding is still veiled. Thus, the tailored engineering of MOP tubes is still limited.The present work unravels a unified mechanism of the tubular formation of MOP materials and enables the tailored engineering of MOP tubes. Three mechanistic methods: self-template route, in situ template route, and additive template route have been elucidated. All three approaches are based on the so-called *double assmebly mechanism*, the noncovalent assembly followed by covalent assembly. In addition, we showed the benefits of ionic MOP tubes with thin shells in the adsorption performance toward model ionic pollutants.

Poster Presentation : **INOR.P-50**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Engineering of Suzuki coupling-based microporous organic network (MON) using Sonogashira coupling-based MON for enhanced sensing

Sang Hyun Ryu, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

This work introduces the first example of the hard template synthesis of Suzuki coupling-based microporous organic polymer(here, termed SUM for simplicity). Recently, the SUM has been prepared and has become one of popular materials. The SUM has shown unique features such as hydrophilic properties due to the defective boronic acid groups and emissive properties. The SUM has been applied for photocatalytic H_2 production and the sensing of harmful compounds. The performance of microporous organicnetwork (MON) is dependent on its morphological structure. It is surprising that as far as we are aware, the hard template synthesis of the SUM has not been reported. Among the MONs, the Sonogashira coupling-based MON (termed SOM for simplicity) has been extensively prepared and usually showed hydrophobic properties. Over the last decade, we has reported the morphological engineering of the SOM. Although we have tried to extend the template synthesis to SUM, the results were not successful. We elucidated the reasons and figured out that the conventional strong bases used in the Suzuki coupling reacted with silica templates to form insoluble inorganic solids ($KHSi_2O_5$). In this work, we report the morphological engineering of SUM using hollow SOM materials. The resultant hollow SOM@SUM showed hydrophilic nature and the enhanced sensing performance for nitrophenols in water, compared with hydrophobic SOM and the non-hollow SUM materials.

Poster Presentation : **INOR.P-51**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Evidence of Wheland Intermediate in the Acetate Assisted C-H Activation by Pd(IV) Active Catalyst Species Studied via DFT Calculations.

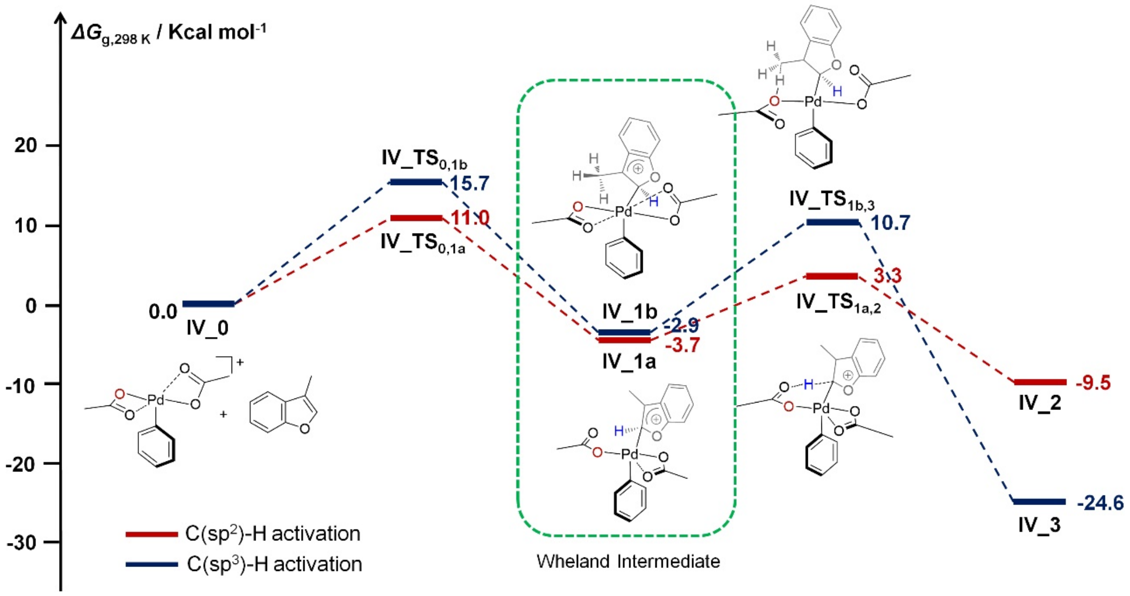
Ji Eun Park, Young Keun Chung[1], Youn Kyung Kang[2,*]

Department of Chemistry, Seoul National University, Korea

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

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

In order to identify the active catalysis species (ACS) of acetate-assisted C-H activation by Pd catalyst for the bisarylation of 3-methylbenzofuran, DFT calculations were performed in the B3LYP/def2TZVP/SDD+ECP level. We considered five ACSs that could be generated from the experimental conditions.: $[Pd^{II}(OAc)(Ph)(PMe_3)]$ (**I**), $Pd^{II}(OAc)_2$ (**II**), $Pd^{II}(OAc)_2PMe_3$ (**III**), $[Pd^{IV}(OAc)_2Ph]^+$ (**IV**)., and $[Pd^{IV}(OAc)_2PhPMe_3]^+$ (**V**). The energy spans for the C(sp^3)-H activation of the five ACS candidates were, 51.4 (**I**), 34.5 (**II**), 75.5 (**III**), 10.7 (**IV**), and 31.4 (**V**) kcal/mol, respectively. Those for the C(sp^2)-H activation were 33.3 (**I**), 18.0 (**II**), 32.0 (**III**), 3.3 (**IV**), and 20.4 (**V**) kcal/mol, respectively, indicating that the cationic Pd^{IV} catalyst without phosphine ligand (**IV**) is the most plausible ACS. This catalyst forms intermediates **IV_1a** and **IV_1b** right before the transition states for the C(sp^2)-H and C(sp^3)-H activations, respectively, that cannot exist in the conventional concerted metalation-deprotonation (CMD) mechanism. Geometrical and Mayor bond analyses of these intermediates clearly show that these are Wheland intermediates manifesting that the reaction mechanism of C-H activation in the bisarylation of 3-methylbenzofuran by **IV** is most likely electrophilic aromatic substitution (SEAr).


ΔG_g,298 K / Kcal mol-1
20
10
0
-10
-20
-30
IV_0
0.0
IV_TS0,1b
15.7
IV_TS0,1a
11.0
IV_1b
-2.9
IV_1a
-3.7
IV_TS1b,3
10.7
IV_TS1a,2
3.3
IV_2
-9.5
IV_3
-24.6
Pd
+
Wheland Intermediate
C(sp2)-H activation
C(sp3)-H activation

Poster Presentation : **INOR.P-52**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Zn-Phthalocyanine-Loaded Microporous Organic Nanoparticles for Dual Chemo-Photodynamic Cancer Therapy

DongWook Kim, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

This work shows that microporous organic network (MON) chemistry can be applied to the dual photodynamic and chemical therapy of cancer cells. While the MON materials prepared by the Sonogashira coupling of conventional organic building blocks have been known to be hydrophobic, in this work, we prepared the water-compatible MON particles for applications to drug delivery materials. Usually, MON materials have been obtained as powders with irregular morphologies and micron sizes. However, the performance of drug delivery materials is dependent on their sizes. It has been well documented that nanoparticles have shown much longer circulation periods because of the lower uptake by the reticuloendothelial system. Due to the enhanced permeability and retention (EPR) effect, nanoparticles have been known to easily access tumors and show high intratumoral accumulation. We engineered the size of MON materials to be nanoscales (55 ± 9 nm) through kinetic growth control. Functional molecules such as Zn-phthalocyanine (ZnPhT) and DOX could be incorporated into MON nanoparticles via chemial and physical strategies. Ultimately, water-compatible and ZnPhT loaded MON nanoparticles could be engineered through size-controlled synthesis and postsynthetic sulfonation of materials. The ZnPhT could be successfully loaded on the sulfonated MON nanoparticles (N-SMONs) through the coulombic interaction between anionic sulfonate and cationic ZnPhT. Due to the microporosity and high surface area, DOX could be loaded efficiently on the ZnPhT/N-SMON nanoparticles. The DOX/ZnPhT/N-SMON showed excellent performance in the dual photodynamic and chemotherapy of cancer cells up to 35% cell viability.

Poster Presentation : **INOR.P-53**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

“Hyper-Cross-Linked Polymer on the Hollow Conjugated Microporous Polymer as an Acidic Heterogeneous Catalyst for Ring-Opening Polymerization of Caprolactone”

Sungjae Choi, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Microporous organic polymers (MOPs) are a recent class of porous materials. Depending on the synthetic methods, the MOP materials were classified into several groups and called by their unique terms. One of the MOP materials is called hypercrosslinked polymer (HCP) and has been prepared by the Friedel-Crafts reaction of building blocks. Another important class of MOP materials is called conjugated microporous polymer (CMP). This work shows the first example of the shape controlled synthesis of another MOP material using the shape controlled MOP materials. The functional performance of MOP materials is dependent on the morphological structure of MOP materials. We has focused on the morphological engieering of CMP materials and has tried to extend from CMP materials to other classes of MOP materials. However, our trials to engineer the morphlogy of HCP materials using silica spheres and $FeCl_3$ catalyst were unsuccessful. This work shows that the hollow HCP materials can be engineered by the hollow CMP materials. Based on the H-CMP@HCP materials, we devloped the hetergeneous catalytic systems for the synthesis of biodegradable, poly(caprolactones). Due to the chemical stability, the H-CMPL@HCP-BP showed excellent recyclability. As far as we are aware, the H-CMP@HCP-BP is the first heterogeneous catalyst for the synthesis of biodegradable PCL.

Poster Presentation : **INOR.P-54**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Post-synthetic modification of microporous organic network based on AB_2 polymerization: Engineering of solid acid catalysts for the chemical transformation of cellulose to soluble cellulose derivatives

Su Kyung Chae, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Recently, the tailored functionalization of microporous organic network (MON) has been an important subject. Since the post-synthetic modification (PSM) strategy has been suggested, there have been creative examples of scientists. However, there has been no examples of the PSM of MON based on the AB_2 polymerization chemistry (the polymerization of AB_2 type monomer). This work shows the first application of the AB_2 polymerization for the PSM of MON. Since the hypothesis of Flory, the AB_2 polymerization has been regarded to generate a unique polymer structure, a highly branched structure. The MON prepared by the Sonogashira coupling has connection defects to generate the minor amount of terminal alkynes. The terminal alkynes can be utilized for the PSM through thiol-yne click reaction to incorporate aliphatic sulfonic acids. However, the absolute amount of terminal akynes is relatively minor. In this work, the terminal akyne in the hollow MON was amplified by the PSM through AB_2 polymerization. Recently, there have been extensive studies on the use of plants as sustainable chemical resources to replace the depletable petroleum. However, the poor solublity of cellulose can be an obstacle in the engineering of functional materials. The chemical transformation of cellulose to soluble cellulose derivatives have attracted significant attention of scientists. For this, efficient solid acid catalysts are required. In this work, using the terminal alkyne enriched MON, we engineered the solid acid catalysts bearing aliphatic sulfonic acids. The solid acid catalysts showed the enhanced catalytic efficiency in the synthesis of soluble cellulose derivatives by 2.7 and 10 times, compared to the commerical Amberlyst-15.

Poster Presentation : **INOR.P-55**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Photophysical Properties and Photoredox Catalytic Activities of Ru(II) Complexes Encapsulated into Metal-Organic Frameworks

Suk bin Yoon, Youngmee Kim[1], Seong Huh[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

Metal-organic frameworks (MOFs) with large well-defined open spaces are ideal host materials for the encapsulation of a range of functional guests. MOFs with negatively charged frameworks are suitable for selectively encapsulating cationic guest ions via simple cation-exchange process with counter-cations present in the channels. Previously, a very large Reichardt's dye (RD) was successfully encapsulated into mesopores of the three-dimensional (3D) InBTB MOF (H_3BTB = 1,3,5-benzenetribenzoic acid). To further explore this new type of optical materials, we tried to prepare new Ru(II)@InBTB MOFs by encapsulating a series of cationic Ru(II) complexes: $[Ru(bpy)_3]^{2+}$, bpy = 2,2'-bipyridine; $[Ru(phen)_3]^{2+}$, phen = 1,10-phenanthroline; and $[Ru(bpz)_3]^{2+}$, bpz = 2,2'-bipyrazine. Their photophysical properties were investigated by photoluminescence (PL) techniques. The photoredox catalytic activities were also investigated for aza-Henry reaction, trifluoromethylation of N-methylpyrrole, and decomposition of methyl orange under visible light irradiation at room temperature. Ru(II)@InBTB MOFs were found to be very stable and highly recyclable photoredox catalytic systems.

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Poster Presentation : **INOR.P-56**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Valence Selectivity of Copper Complex by Counteranion Size Effect

Eun su Chae, Jang Hoon Cho, Hong In Lee[*]

Department of Chemistry, Kyungpook National University, Korea

Metal valence state can regulate the complex activity to act as oxidant or reductant, and many kinds of metal valence state depend on counteranion or ligand valence state. In case of copper complex, they usually show divalent copper, and rarely show monovalent copper. Because of this reason, many copper complexes which have either perchlorate ion or bromine perchlorate ion reported as divalent. So, valence selectivity by counteranion size effect is important at copper complex to make monovalent copper complex easily. In this study, we have synthesized a new bisquinoline schiff base ligand which forms monovalent copper complex, [Cu(EbQMA)]ClO_4, and forms divalent copper complex, [Cu(EbQMA)Br]ClO_4.

Poster Presentation : **INOR.P-57**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Three Platinum Complexes with Tetradentate Dipyridine Ligands and Their Application As Electroluminescent Materials

Suk-Hee Moon, Youngjin Kang[1,*], Ki-Min Park[2,*]

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[1]*Division of Science Education, Kangwon National University, Korea*
[2]*Research Institute of Natural Science, Gyeongsang National University, Korea*

Our interest in developing highly efficient blue triplet emitters for application in PHOLEDs has prompted us to synthesize tetradentate-ligand-based Pt(II) derivatives, as well as to investigate their photophysical and electroluminescent characteristics. To date, three phosphorescent platinum complexes based on C^N chelating 2,3'-dipyridine ligand have been designed and synthesized. The structures of all the complexes were confirmed by various spectroscopic methods, including X-ray diffraction analysis. All complexes emit bright blue to sky blue phosphorescence with λ_{max} = 460 nm ~ 490nm. Blue phosphorescent organic light-emitting diodes (PHOLEDs) using all complexes have been successfully fabricated. An external quantum efficiency of 17.6% (maximum) and 17.3% (at 100 cd/m^2) are observed. Moreover, under a doping level of 50 wt%, white organic light-emitting diodes (WOLEDs) have been also successfully fabricated. It exhibits pure white emission with the CIE coordinates (x, y) of (0.32, 0.34). Here, we describe the results of our investigation on the preparation, crystal structure, and electroluminescent characteristics of square-planar Pt(II) bearing a C^N chelated dipyridine ligand. Moreover, we also discuss the effects of substituents of a linker or main ligand on the performance of PHOLEDs and white organic light-emitting diodes (WOLEDs).

Poster Presentation : **INOR.P-58**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Comparison of various crystal structures of hexaaquadivalentmetal bis((E)-4-((4-(dimethylamino)phenyl)benzenesulfonate), $C_{28}H_{40}N_6MO_{12}S_2$ ($M=Mn^{2+}$, Ni^{2+}, Mg^{2+})

Garam Park, In-Hwan Oh[1,*]

Radiochemistry department, Korea Atomic Energy Research Institute, Korea
[1]*Neutron Science Division, Korea Atomic Energy Research Institute, Korea*

Recently, inorganic-organic system attracts many attentions because of their unique interesting physical properties, for example, low-dimensional magnetism, photovoltaic effects and thermoelectrics [1,2,3,4,5]. To get an adequate systme, we have tried to synthesize various inorganic-organic systems including $(C_6H_5CH_2CH_2NH_3)_2MCl_4$ ($M=Cu^{2+}$, Mn^{2+}, Co^{2+}) and M-Methylorange (MO) ($M=Mn^{2+}$, Ni^{2+}, Mg^{2+}) [6,7,8,9,10,11]. In this work, we will show Mn-, Ni- and Mg-Methylorange sysmtes and compare in the crystal structural point of view.

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Poster Presentation : **INOR.P-59**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Kinetically Controlled Ag^+-Coordinated Supramolecular Polymerization

Jeong Sang Oh, Jong Hwa Jung[1,*]

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

Bipyridine-based ligand (**1G**) possessing hydrazine and glycine moieties at the alkyl chain groups have been synthesized. The supramolecular polymer **1** (8 mM) was prepared by functional building block **1G** (8 mM) with 1.0 equiv. of $AgNO_3$ in water. The supramolecular polymer **1** was characterized by time- and temperature-dependent UV-Vis analysis and atomic force microscopy (AFM). This supramolecular polymer **1** kinetically assembles into thermodynamically stable aggregate. The plot of the time-dependent UV-Vis spectral changes of supramolecular polymer **1** showed a non-linear sigmoidal transition. The long lag time in the UV-Vis observations implies the existence of the kinetic aggregate. And heating curves of supramolecular polymer **1** obtained by plotting of temperature-dependent UV-Vis spectra at 345 nm was also found to be clearly non-linear sigmoidal shape, indicative of a cooperative supramolecular polymerization mechanism. And spectral changes of temperature-dependent UV-Vis were slightly red-shifted when heated from 20℃ to 80℃. Additionally, the transparent solution became a colloidal suspension upon addition of $AgNO_3$ (1.0 equiv.) to a **1G** (8 mM) solution. According to AFM observations, the supramolecular polymer **1** with 1.0 equiv. of $AgNO_3$ showed the fibers.

Poster Presentation : **INOR.P-60**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Development of hybrid nanomaterials and self-assembly

Su Hyeon Park, Cheongwon Bae, Jaedeok Lee, Juyeong Kim*

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Hybrid nanomaterials, composed of a metal nanoparticle core and a higher-order construct shell, can have multi functions and synergistic effects. We develop a synthetic method to combine metal nanoparticle cores and metal-organic framework shells. As a model system, we chose shape-anisotropic gold nanoparticles and zeolitic imidazolate frameworks (ZIF-8). We investigated the product formation by varying precursor concentration, reaction temperature, particle concentration and shape. The shell thickness and coverage on the nanoparticle core could be controlled with those factors, which will help to design innovative hybrid nanomaterials for molecular sensing.

Poster Presentation : **INOR.P-61**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Theoretical Perspectives in CONY-Grubbs Catalysts

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The control of the electronic and steric properties of the N-heterocyclic carbene ligands is taken as a crucial factor that greatly affects the efficiency and selectivity of Grubbs catalyst in olefin metathesis. Thus, starting with changing functional groups of the representative cyclic diaminocarbene, there are several examples to introduce the uncommon NHC such as cyclic (alkyl) amino carbene (cAAC), diamidocarbene (DAC), and abnormal NHC, in the Grubbs catalyst. Among these, cAACs ligated Grubbs catalysts (Bertrand-Grubbs catalysts) have attracted much attention since cAACs can effectively stabilize the ruthenium complex and show remarkable reactivity to ethenolysis. However, Bertrand-Grubbs catalyst derivatives only change the steric properties and they cannot change the electronic properties effectively. Thanks to the study by Togni and Sigman groups, we now know that the electronic properties of ligand and metal complexes strongly affect to efficiency and selectivity of Grubbs catalyst in ethenolysis. For these reasons, we designed the CONY-Grubbs catalysts. Because coumaraz-2-on-4-ylidene (CONY) is a tunable N-heterocyclic ligand platform, we assume that it can change the electronic properties of the ruthenium complexes directly. By DFT calculation, we also discovered that the HOMO and LUMO energies of CONY-Grubbs catalysts change in the right direction, as demonstrated by Togni and Sigman groups.

Poster Presentation : **INOR.P-62**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Ammonia Synthesis by Penta-Pyridine Molybdenum Complex

Jeongmin Cha, Hyunchul Kwon[1], Hayoung Song, Eunsung Lee*

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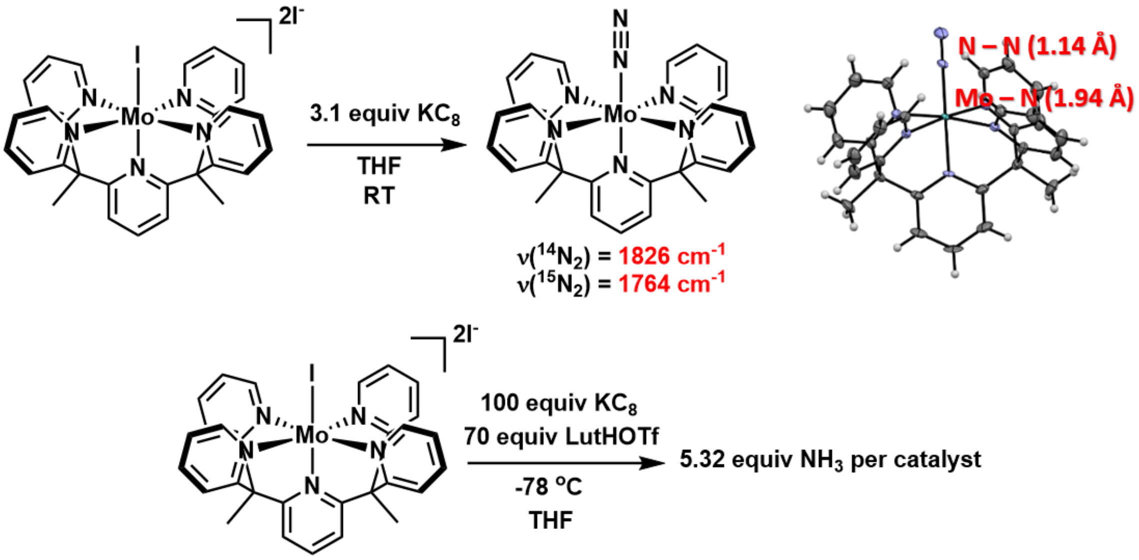
[1]Chemistry, UC Berkeley, United States

Since the first discovery of dinitrogen complex by Allen and Senoff, employing dinitrogen(N_2) as a chemical stock has been stimulating synthetic inorganic chemists. The most fascinating reaction for N_2 is synthesizing ammonia(NH_3) under benign condition, otherwise the synthesis of ammonia requires a huge energy from Haber-Bosch process. In 2003, the Schrock group demonstrated a well-defined system where bulky molybdenum system catalytically converted N_2 to NH_3 with mild reagents. Since then, numerous homogeneous catalysts for N_2 reduction have been reported, of which the Peters group represents an iron system and the Nishibayashi group represents molybdenum systems. Here, we report NH_3 synthesis by a penta-pyridine molybdenum system. The N_2 complex was characterized crystallographically and spectroscopically, in which the data indicated the N_2 ligand was highly activated. The catalytic reaction was also attempted for being optimized for electron and proton sources.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **INOR.P-63**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Single-particle plasmonic imaging of multistep nanoscale sulfidation of Ag nanocubes by L-cysteine

Hyuncheol Oh, Hyunjoon Song*

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

The generation of complex nanostructures to obtain novel characteristics and improved performance has been achieved by coupling multiple nanoscale reactions. Because reactions at nanometer scale directly govern the morphology of nanostructures, understanding the reaction mechanism is critical to precisely control the morphology and, eventually, the physicochemical properties of the materials. However, because of the ensemble-average effect, investigating the reaction mechanism at the bulk level does not provide sufficient information. In this study, we investigated the overall sulfidation reaction mechanism that occurred on individual silver nanocubes in real time at high temperature. Using the single-particle dark-field imaging technique, three discrete steps of the sulfidation reaction were clearly resolved in the profiles of plasmon peak shift and intensity change of individual particles according to time progress: (I) reactant diffusion to silver surface by passing through ligand barrier, (II) silver sulfide formation by C-S bond cleavage of cysteine molecules, and (III) diffusion of silver atoms in silver sulfide layer until the complete formation of silver sulfide. By a combination of simulation and control experiments, physical constants were derived for each step, which is completely hidden in the ensemble measurements.

Poster Presentation : **INOR.P-64**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of bis-pyridinium nicotinamide for phosphate detection

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

As the importance of negative ions increases in many fields, the development of negative ions receptors and sensors has been studied in various fields[1]. There is an interest in developing molecules that can selectively and sensitively recognize anions.Therefore, we synthesized bis-pyridinium nicotinamide to detect phosphate anions.This compound, which is expected to detect phosphate, was synthesized with m-Xylylene dibromide and nicotinamide and was found to be clear on NMR.Since there are very few reports of nicotinamide-based phosphate-sensing complexes, this compound attempts to titrate NMR, form it into a membrane type, and combine it with an electrode to measure the amount of phosphate anion detected, making sure it is well-detected[2].References1.(a) Brzo’zka,Z. In “Comprehensive Supramolecular Chemistry”; Atwood, J. L., Davies, J.E.D., MacnNicol, D.D., Vögtle, F., Suslick, K, S., Eds.; Pergamon: Oxford, 1996; pp 187-212 (b) “Chemosensors of Ion and Molecular Recognition”; Desvergne,J.-P., Czarnik, A. W., Eds.; Kluwer: Dordrecht, 1997; Vol 492.2.“Phosphate-selective polymer membrane electrode”, Scott A. Glazer, and Mark A. Arnold, Anal. Chem., 1998, 60 (22), pp 2540-2542.

Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Oxygen atom transfer: a mild and efficient method for generating iminyl radicals

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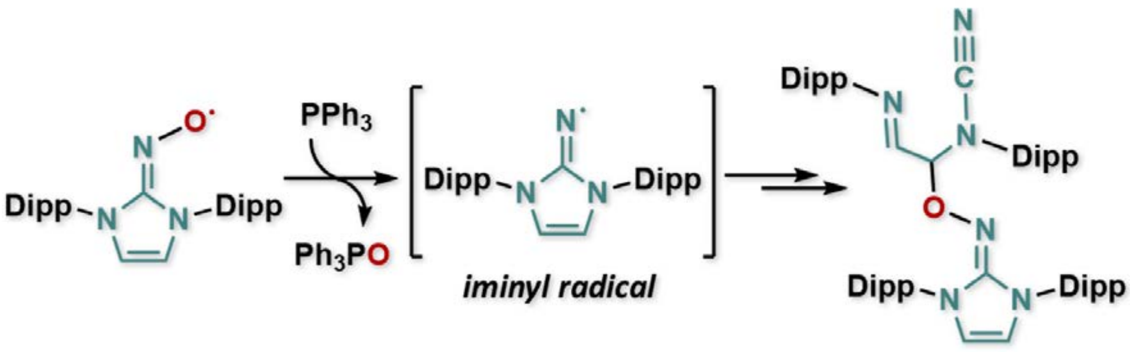
Nitrogen-centered radicals are of broad interest because they provide a means for introducing nitrogen atoms into various substrates. Along with their aminyl analogues, iminyl radicals have been used to construct nitrogen containing molecules (e.g., N-heterocycles) and applied in C–N bond forming reactions. Although iminyl radicals are often generated by subjecting their oxime derivatives to microwaves, UV irradiation, or high temperatures, relatively mild conditions that accompany photocatalyzed single electron transfer processes have been recently reported. Herein we report a new method for forming iminyl radical intermediates *via* oxygen atom transfer.[1] Treating iminoxyl species with oxygen acceptors such as PPh_3 resulted in oxygen atom transfer and afforded the corresponding iminyl radicals. DFT calculations revealed that association between the oxygen atom acceptors and the iminoxyl species results in the formation of adducts during the reaction. Subsequent dissociation is accompanied with homolytic cleavage of the N–O bond and generates iminyl radicals with spin densities that are localized on exocyclic nitrogen atoms.Reference[1] Y. Kim, C. W. Bielawski, E. Lee*, *Chem. Commun*. **2019**, *55*, 7061.



Poster Presentation : **INOR.P-66**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Detection of Phosphate anion through Membrane Electrode and NMR titration based on Diimidazolium complex.

Jin Seong Oh, Young Il Kim, Jungseok Heo[1,*]

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

As the Importance of anionic species increase in biology, catalysts and the environment, we are interested in developing molecules that can selectively recognize and detect these negatively charged ions. The development of receptors and sensors for anions in nature is emerging as an important research area. Sensors for various ions have been studied, and here we have synthesized a phosphate sensitive diimidazolium complex that has good selectivity for phosphate anion. Though many reported phosphate sensors include Imidazolium arm, there are few reports, to the best of our knowledge, of Imidazolium based phosphate sensing complexes derived from a 1-butylimidazole. 1,3-bis(dibromomethyl)benzene and 1-butylimidazole were synthesized to a ligand having two imidazolium sites. And Through these compounds we attempted NMR titration and made this into a membrane type and combined it with electrode to measure the amount of sensed phosphate anion.

Poster Presentation : **INOR.P-67**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Series of g-C3N4@MxWO3 (M=K, Na) nanocomposites as smart window coating for energy savings and environmental decontamination

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Multifunctional smart window coating can achieve two function at the same time, also it is environmental friendly. MxWO3 (M=K, Na) were synthesized by two steps. The composite films showed nice UV absorption and NIR shielding properties. The photocatalyst activity was improved by using two kind catalyst. The photocatalyst activity was mainly depend on Z-scheme.The new g-C3N4@MxWO3 (M=K, Na) composites not only showed promising harmful UV light absorption, high VIS light brightness, excellent NIR light induced heat insulation, but also nice toxic HCHO/toluene photodecomposition property, indicating their brilliant prospect in both of energy saving and environmental decontamination, which can applied in smart window area. But the stability need to be improved. And the absorption of solar light need to improve. Keywords: g-C3N4@MxWO3, Z-scheme heterostructure, Multifunctionality, NIR shielding,Photocatalytic activity

Poster Presentation : **INOR.P-68**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Mechanism study of direct C-H arylation of Pd(II)/Pd(0) nanoparticles using diaryliodonium oxidants.

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C-H arylation that converts C-H bond to useful C-Ar bond has been studied actively in heterogeneous catalysis. In particular, hetero-aromatic compounds such as indole and benzofuran, which are used as building blocks for drug or natural products, have been widely studied. The traditional way of C-H arylation was to use C-C coupling reactions, but recently, diaryliodonium oxidants have been used to selective C-H arylation. Glorius and co-workers reported that selective C-H arylation using diaryliodonium salts and proposed mechanistic studies proceeding via a Pd(0)/Pd(II) systems by kinetic studies. However, the precise structure of active species have not yet been identified. In this presentation, we report direct C-H arylation of hetero-aromatic compounds using Pd(II)/Pd(0) nanoparticles. X-ray absorption fine structure (XAFS) has been used to determine the coordination chemistry of active species.

Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

A New Visible Light Photocatalyst for Lignin Biomass: Cadmium sulfide Nanoparticles with silver compound

Hyeonji Yoo, Hyun Sung Kim[1,*]

chemistry, Pukyong National University, Korea

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

Bio energy is the energy obtained by using biomass as a fuel and is an alternative energy that can be used as a material for biological resources. Among them, lignin is an easily obtainable material from wood and is being studied for use as fuel. One of the tasks of depolymerizing lignin to noble metal aromatics is to selectively cleave the rich C-O bond of the β-O-4 bond. In this study, we attempted to decompose the C-O bond of β-O-4 alcohol using a single catalyst. In addition, the difference in efficiency is investigated by forming Ag_2S in CdS used as a lignin decomposition catalyst. Ag_2S is easily formed on the surface by adding Ag^+ ion to CdS and expects a different effect from single CdS.

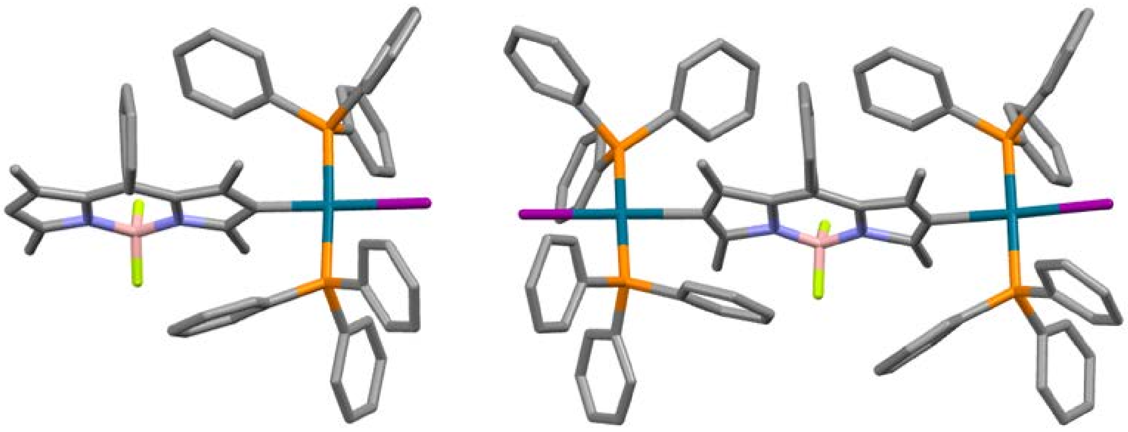
Poster Presentation : **INOR.P-70**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Bodipy based Palladium complexes formed via Oxidative Addition Reaction

Gajendra Gupta, Chang Yeon Lee*

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

Abstract: Boron-dipyrromethene, commonly known as BODIPY, are well known fluorescent molecules used for several important applications including biological labelling and photosensetizers for photodynamic theraphy studies.[1] The BODIPY ligand can be fine tuned, keeping its physical and chemical properties intact, for certain important applications.[2] Herein, we have syntheiszed two new Pd based mono-Iodine and di-Iodine BODIPY complexes through oxidative addition reaction. The complexes were fully characterized using different analytical techniques including SCXRD (figure below). The presence of one and two heavy Iodine atom is being utilized to realize its biological activity through photodynamic theraphy studies.Figure: Molecular structures of mono-Pd (L) and di-Pd (R) inserted BODIPY complexes.References: 1.Jianzhang Zhao et. al., Chem. Soc. Rev. 2015, 44, 8904.2.G. Gupta and C. Y. Lee et. al., Chem. Commun. 2016, 52, 4274; Chem. Eur. J. 2017, 23, 17199; Inorg. Chem. 2017, 56, 4615; Inorg. Chem. 2019, 58, 8587; Dyes and Pigments 2019, 170, 107576.



Poster Presentation : **INOR.P-71**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Reversible Ammonia Uptake in an Imidazolium-based Metal Organic Framework at Room Temperature

Jaechul Lee, Dae-Woon Lim[1,*], Kimoon Kim, Eunsung Lee[*]

Department of Chemistry, Pohang University of Science and Technology, Korea
[1]*Chemistry, Kyoto University, Japan*

Metal–organic frameworks (MOFs) have attracted great interest due to their potential applications such as catalysis, gas storage, and separation of molecules. However, there has been less studied on the utilization of imidazolium functionality in MOFs for various applications. In this research, we designed a new imidazolium ligand with pyrazolate as a metal binding sites and synthesized cobalt based 3D MOF from the ligand. The reversible ammonia capture using the framework was demonstrated by gas sorption experiments. Furthermore, we demonstrated the control of NH_3 adsorption affinity and uptake capacity of framework by simple ion substitution in a post synthetic manner.

Poster Presentation : **INOR.P-72**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Rapid Adsorption and Removal of Sulfur Mustard with Zeolitic Imidazolate Frameworks ZIF-8 and ZIF-67

Son Yerim, **Hyun Sung Kim**[1,*]

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

This study applies two isostructural zeolitic imidazolate frameworks (ZIF-8 and ZIF-67) to rapidly adsorb and remove sulfur mustard (HD), a chemical warfare agent. Because HD is extremely toxic, some of this studies were conducted using an HD simulant, 2-chloroethyl ethyl sulfide (CEES), to understand the effect of solvent polarity on adsorption. Further, CEES and real HD were subsequently adsorbed and removed from aqueous solution using ZIF-8 or ZIF-67. The adsorption abilities of ZIF-8 and ZIF-67 positively correlated with the polarity of the solvent. In addition, 97% of CEES (2.5 mg in 1mL) was rapidly adsorbed by ZIF-8 and ZIF-67 within 1 min at 25 ^{o}C in a 9:1 (v/v) water/ethanol solution. ZIF-8 and ZIF-67 were also successfully fabricated on cotton, which was removed more than 95% of contaminants from substrates contaminated with the HD simulant. We believe that this work will encourage the developement of ZIFs for chemical warfare defense.

Poster Presentation : **INOR.P-73**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of the high functional supramolecular building block

Seok gyu Kang, Jong Hwa Jung[1,*]

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

I present on the synthesis of high functional building blocks formaking the self-assembled supramolecular polymer. OPE-1 as a supramolecular building block is prepared by a multistep synthesis. The essential building block OPE-5 for the elongation of OPE chains was prepared via alkylation and iodination of 1,4-dihydroquinone. The polar nature of the alkyloxy groups turns out to be very beneficial to subsequent column chromatographic separations. Next, monomeric phenyl acetylenes OPE-4 and OPE-3 were readily synthesizedby cross-coupling and K_2CO_3 desilylation reactions. Finally, I synthesized the trimer OPE-1 using the divergent kidney pathway and confirmed it by nuclear magnetic resonance spectroscopy, mass spectroscopy, and elemental analysis.

Poster Presentation : **INOR.P-74**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Investigation of CO_2 capturing capacity for various amino acids incorporated MOFs

Miyeon Kim, Jiwon Kim, Se-In Kang, Chaeyeon Yoo, Chang Yeon Lee*

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

Metal-organic frameworks (MOFs), constructed via coordination bond between inorganic secondary building units and multidentate organic ligand units, have emerged as an innovative porous material. Their enormous surface area, tunability of pore size and ordered structure enable us to demonstrate the various applications including gas storage, separation, sensing, drug delivery, and catalysis. Especially, Zr-based MOFs are more suitable for gas storage, due to their high thermal, chemical and mechanical, as well as water-stability.[1]Recently, Carbon dioxide (CO_2) capture is getting more attention due to the continuous global warming problem. The conventional CO_2 capture method, however, has disadvantages that the formation has corrosive character and high regeneration energy is required. For this reason, several MOFs have recently been used for CO_2 capture.[2] In this research, we aimed to maximize the efficiency of CO_2 capture through amino acid incorporated Zr-MOFs obtained via SALI. Modified Zr-MOFs exhibit enhanced performance compared to the parent MOFs.References1)Pravas Deria and Wojciech Bury, Chem. Commun., 2014,50, 1965-19682)Trickett, C. A. et al, Nat.Rev. Mater, 2017, 2, 17045

Poster Presentation : **INOR.P-75**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Partial Pt^{2+} insertion into ZIF-8 nanocubes toward the formation of face-centered-tetragonal PtZn intermetallic nanoparticles

Taehyun Kwon, Sunghyun Lim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Pt-based electrocatalysts have been widely used in anodic oxidation of fuel and cathodic oxygen reduction reaction. Several researches adopted the incorporation of earth-abundant 3d-transition metal elements with Pt, forming alloy electrocatalysts, in order to reduce the usage of Pt. In particular, atomically ordered (intermetallic) nanoparticles with well-defined crystal structures showed high electrocatalytic activity and durability with dissolution-resistant surface. In this work, we present direct conversion of Pt^{2+} ion-inserted ZIF-8 nanocubes toward face-centered-tetragonal PtZn (fct-PtZn) nanoparticles supported on hollow nitrogen-doped carbon nanocage via thermal annealing under reductive condition that exhibit superior catalytic activity in the fuel oxidation reaction.

Poster Presentation : **INOR.P-76**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Morphology transformation in $Cu_{2-x}S/Ag_2S$ nanoplates induced by surface energy modulation and phase miscibility

Taekyung Kim, Jongsik Park, Yongju Hong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

In the synthesis of nanoparticles, it is difficult to control the growth of nanoparticles having regiospecifically arranged multiple compositions. These nanocrystals with multiple components usually have heterointerfaces in which the lattice mismatch is one of the critical determinants of the surface energy modulation. To date, heterointerfaces have been considered to be static and the dynamic movement of components within the multiple components of a materal has not received a great attention although the dynamic movement of one component within multicomponent materials may update the interpretation of the catalytic behaviors of these materials and lead to new concepts for nanostructure synthesis. Herein, we witnessed that dynamic movement of components through the hetero-interface; remarkable cation migrations within the sulfide matrix can be induced by surface strain modulation. We further show the dynamic hetero-interface within a nanostructure with Janus $Cu_{2-x}S/Ag_2S$ nanoplates can be influenced by the degree of phase mixing and segregation between components.

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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **INOR.P-77**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

The transition metal doping of IrRu shell of $Cu_{2-x}S$@IrRu nanoparticles for oxygen evolution reaction in acidic media

Jinwhan Joo, Ye Ji Park, Kwangyeol Lee[*]

Department of Chemistry, Korea University, Korea

We have recently reported that the cactus-like $Cu_{2-x}S$@IrRu, serving as a bifunctional catalyst, exhibits excellent catalytic activity and stability toward the hydrogen evolution reaction and oxygen evolution reaction. For the OER, the oxidation of the surface IrRu phase is inevitable, and thus the atom packing motif of the surface oxide is of key importance to the catalytic activity and stability. It has been previously demonstrated that the presence of vacant sites in the metal oxide is crucial to the stability enhancement of metal oxide toward OER. Therefore, we have investigated the doping of Cr, Mn, Fe, Co, and Ni to engineer the vacant sites of IrRu phase in order to develop OER catalysts with further enhanced catalytic activity and stability. Among the transition metal dopants tested, Mn dopant dramatically improves the electrocatalytic activity of IrRu catalyst. Herein, we report our efforts to understand the underlying principle behind Mn-assisted performance boosting the catalytic performance of IrRu oxide.

Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis of Carbazole Conjugated Salen-In Systems and Their Photopysical Properties

Chan Hee Ryu, Sang Woo Kwak[1], Myung Hwan Park[2,*], Kang Mun Lee[*]

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[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*
[2]*Department of Chemical Education, Chungbuk Natioanl University, Korea*

Novel carbazole-conjugated salen–In complexes (**Cz1** and **Cz2**) were prepared and fully characterized by multinuclear NMR spectroscopy, elemental analysis, and high-resolution mass spectrometry. The photoluminescent spectra of **Cz1** and **Cz2** showed broad emission bands centered at 459 nm and 507 nm in THF, respectively, which are typical for CT transitions. In particular, **Cz1** showed 8-fold enhanced quantum efficiency than **Cz2**, with a 3-fold higher photoluminescence quantum yield than that of the salen−In complex without the carbazole parts. Such the enhanced luminescence efficiency of **Cz1** originated from efficient radiative decay based on the ICT transition between the salen−In moieties and carbazole parts, as well as its structural rigidity in conversion process between the ground (S_0) and excited (S_1) states. In other words, **Cz2** exhibited the low quantum yield due to its structural fluctuation, which is free rotation of both the appended carbazole moieties and bridged phenylene rings in conversion between the S_0-and S_1-structures. In addition, these salen–In complexes exhibited high thermal (T_{d5} = 367 °C for **Cz1** and 406 °C for **Cz2**) and electrochemical stability.

Poster Presentation : **INOR.P-79**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Observation of new phases between K and Cd under ambient CO2 pressure.

Kang Yeong Kim, Young-Uk Kwon[1,*]

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

The formation of A2M(CO3)2 is usually found between alkali metal (A) and alkaline earth metal (M). Alkaline earth metal can be replaced with d-block element such as Fe, but requiring high pressure and temperature. Here, the carbonation of K2CO3-added CdO system has been studied under ambient pressure of CO2 and we observe new double carbonate phases between K and Cd. The new phase (2) starts to be formed from 230 °C and transformed into other new phase (1) with increasing temperature. Simulating several XRD patterns based on other structure of double carbonates containing alkali earth metal and comparing with these, we identify the crystal structure of phase 2 were similar to nyerereite and its chemical formula is K2Cd(CO3)2.

Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis of AuPt@RuO$_x$ core@shell ternary nanowires and their morphology dependent performance toward the oxygen evolution reaction

Heesu Yang, Taehyun Kwon, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

With the increasing demand for sustainable energy sources, water splitting technology has become one of the promising routes to overcome environmental issues. Among them, Ru-based catalyst is one of the most promising materials in OER reaction, while its stability in acidic media is still a challenging issue. We recently found that the incorporation of Pt contents into RuO$_x$-based nanoparticles resulted in the improved stability as well as activity toward the OER in acidic media. On the other hand, nanowires of precious metals as 1-D nanostructures established themselves as promising electrocatalyst due to their multiple anchoring points among themselves ensuring the thermal stability. Herein we show the synthesis of core@shell nanowires geared toward efficient Pt doping of the RuO$_x$ and the greatly enhanced activity and durability of them toward OER.

Poster Presentation : **INOR.P-81**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Evaluation of functional magnesium silicate synthesis using diatomite as filter aids.

HongBeom Shin, Kyung Min Yoo, Sungho Park[1,*]

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

The purpose of this study is to evaluate the porous substance magnesium silicate by chemical adsorption of impurities (eg, KOH, H_2O) contained in polyols, and its purification ability is correlated with the particle size and surface area of magnesium silicate. As the amount of nanoparticles produced increases, the purification ability is improved, but the washing time and the purification filtration time increase because of blocking the filter paper. Therefore, diatomite with excellent physical adsorption ability and larger particle size than magnesium silicate was used as filter aids.Magnesium silicate were synthesized using a magnesium source ($MgSO_4$, $Mg(NO_3)_2$) and sodium silicate (No.2 – Na_2O:SiO_2=1:2.7). To synthesize a functional magnesium silicate, in-situ method and ex-situ method were used. The in-situ method is the synthesis of magnesium silicate with diatomite directly from one pot. The ex-situ method is a method of mixing the synthesized magnesium silicate powder by washing, drying and grinding process with diatomite powder. Since the in-situ method has a partially coated diatomite with magnesium silicate and the forming fewer nanoparticles blocking the filter paper than the ex-situ method, made the purification-rate of the in-situ method faster than ex-situ. However, it was difficult to remove the byproduct (Na_2SO_4) in diatomite. The result of this study indicate that in-situ magnesium silicate synthesis method diatomite as a filter aid can reduce the amount of nanoparticles that block the filter paper, thereby shortening the purification time and improving productivity.

Poster Presentation : **INOR.P-82**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

New Germanium complexes for thin film application

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[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

In order to deposit conformal films in the high aspect ratio trench and via structures in future high-density phase-change memory devices, suitable atomic layer deposition (ALD)/ chemical layer deposition (CVD) precursors are needed. We have successfully synthesized novel germanium (II) precursors containing β-diketonate and aminoalkoxide ligands. A series of germanium complexes were prepared to examine the effect of coordination ability of the aminoalkoxide ligand in these complexes as well as potential germanium precursors and these complexes could potentially serve as precursors for thin-film applications. Stability studies were conducted to investigate the suitability of the precursors for use as ALD/CVD precursors for device manufacturing. All the complexes were characterized by H-NMR spectroscopy as well as elemental and thermos-gravimetric (TG) analyses. Germanium complexes showed that the complexes display high volatility and thermal stability and these complexes could potentially serve as precursors for thin-film applications.

Poster Presentation : **INOR.P-83**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Construction and Characterization of Metallocages Based by Tantalum(V) Cluster.

Minji Jeong, Younghun Kim, YeonJeong Lee[1], Philjae Kang[2], Moon-gun Choi*

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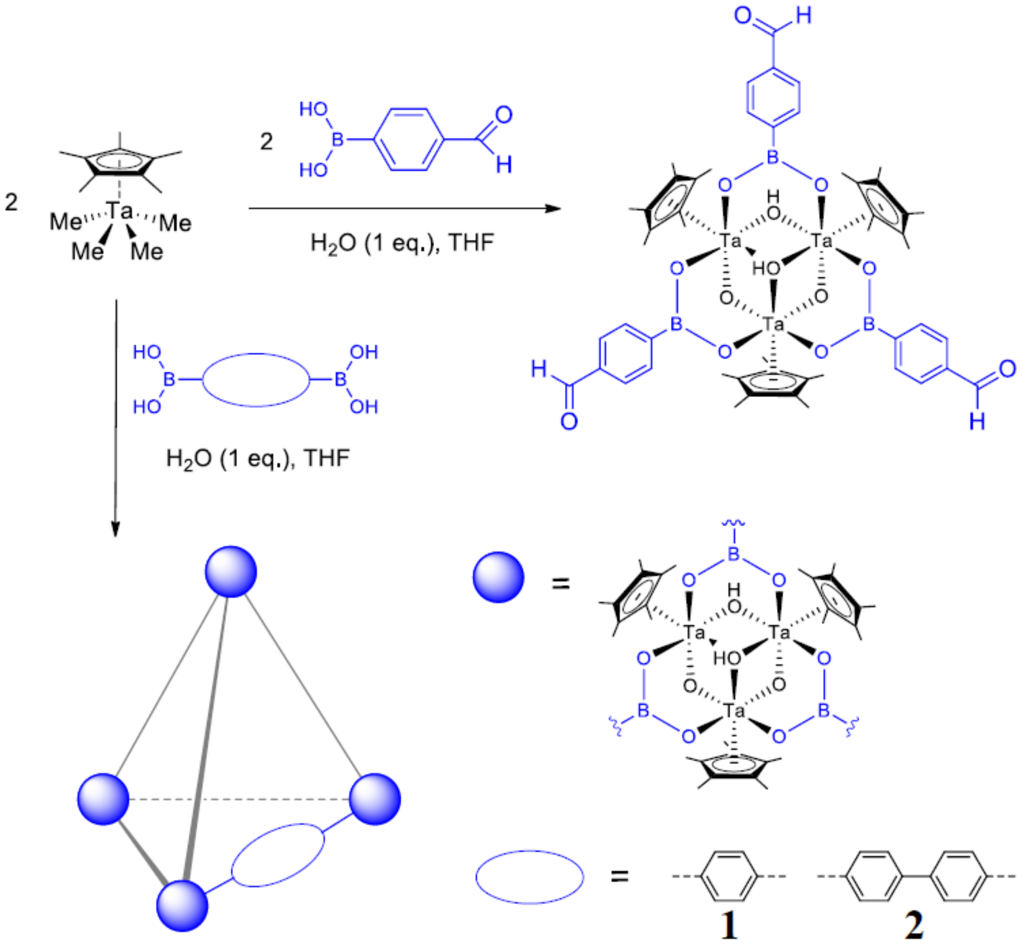
[1]*Yonsei University, Korea*
[2]*Department of Chemistry, Hallym University, Korea*

A neutral metallocavitand and tetrahedral metallocages containing trimetallic tantalum clusters are prepared by a coordination self-assembly of [Cp*Ta(Me)$_4$Cp* = η^5-C_5Me_5) and various boronic acids. Each compounds are characterized by ^{1}H NMR and their 3-D structures are revealed by single crystal X-ray diffraction (SC-XRD). The metallocavitand shows a cup-like shape and metallocages show a tetrahedral shape with a type of V_4E_6 (V= vertex, E= edge). In detail, metallocages are composed of {[Cp*Ta]$_3$(μ^2-OH)(μ^2-O)$_2$(μ^3-OH)} as a vertex and boronate ligands as an edge. Additionally, each cages has different size of pores and packing structures depending on the length of ligands.


2
Me
Ta
Me
Me
Me
2
HO
B
HO
O
H
H2O (1 eq.), THF
HO
B
HO
OH
B
OH
H2O (1 eq.), THF
=
=
1
2

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Longitudinal Strain Engineering of $Cu_{2-x}S$-based Nanosandwich

Sunghyun Lim, Jongsik Park, Taehyun Kwon, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Fabrication of complex hetero-nanostructures via post-modification methods opens a new horizon in nanomaterial-based research applications. In particular, cation exchange (CE) is a central strategy for manipulating the composition and morphology of as-synthesized nanocrystals (NCs). The surface strain engineering of nanoparticles has been extensively investigated to change the electronic states of nanoparticles, with specific aims to induce novel optical and catalytic properties. Herein, we show that slow incorporation of Fe at the exposed surfaces of hexagonal $Cu_{2-x}S$ forms Cu_5FeS_4 and $Cu_{2-x}S$ along the z-axis direction induces the surface strain. We believe that this synthetic concept can be further expanded to other material phases so as to form highly sophisticated multiphasic, and well-designed 3-dimensional nanoparticles that are geared to possess exciting physicochemical properties.

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Poster Presentation : **INOR.P-85**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of Porous Pt-based Nanoparticles as Catalysts for Selective Hydrogenation Reactions

Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Selective hydrogenation of compounds is one of the main issues in organic synthesis. While conventional heterogeneous catalysts have excellent activity, most of them have poor selectivity. Therefore, selectivity of nanocatalysts can be improved by controlling their surface energy, which depends on chemical composition and coordination nature of the surface. Herein, we report the synthesis of porous Pt-based nanoparticles as catalysts for hydrogenation reactions. The prepared porous Pt-based nanoparticles exhibit superior selectivity for hydrogenation reactions of unsaturated hydrocarbons.

Poster Presentation : **INOR.P-86**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Non-enzymatic Glucose Biosensor Utilizing High Purity TiO_2 Nanoparticles Deposited Directly by Thermal Plasma

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chemistry, Daejin University, Korea
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This study proposes a non-enzymatic glucose sensor fabricated by synthesizing high-purity TiO_2 nanoparticles in thermal plasma and depositing it directly on a substrate and depositing a Chitosan-Polypyrrole conductive polymer films by electrochemical method. The structural properties of the deposited TiO_2 nanoparticles were analyzed by Transmission Electron Microscope (TEM), X-ray Diffraction (XRD), and Dynamic Light Scattering system (DLS). The chemical composition and structural properties of the TiO_2 nanoparticle layer and the conductive polymer films were confirmed by X-Ray Photoelectron Spectroscopy (XPS) spectra, Scanning Electron Microscope (SEM) and Atomic Force Microscope (AFM). The glucose detection characteristics of the fabricated biosensor were determined by Cyclic Voltammetry (CV). High purity TiO_2/CS-PPy biosensor showed 1.5 times higher sensitivity of glucose oxidation current from 1.5mA to 2.3mA compared to sol-gel TiO_2/CS-PPy biosensor. In addition, the oxidation current was about 2.2 times higher than that of CS-PPy conductive polymer films biosensor, from 1.05mA to 2.3mA. The high purity TiO_2/CS-PPy biosensor showed excellent selectivity and reactivity with glucose concentration.

Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Development of a Lower Energy Photosensitizer for Photocatalytic Water or Carbon Dioxide Redcution: Modification of Squaraine Dye in Ternary Hybrid System (Dye/TiO_2/Re(I))

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Department of Advanced Materials Chemistry, Korea University, Korea

Red light-sensitized squaraine (**SQ**) dyes were developed and incorporated into dye-sensitized catalyst (DSC) with the formula of **SQ**/TiO_2/Cat, and their efficacies were evaluated in terms of performance on either water or carbon dioxide reduction. Pt nanoparticles or *fac*-[Re(4,4′-bis-(diethoxyphosphorylmethyl)-2,2′-bipyridine)$(CO)_3Cl$] were used as each catalytic center within the DSC frame of **SQ**/TiO_2/Pt (Type I) or **SQ**/TiO_2/Re(I) (Type II). In order to convey the potential utility of **SQ** in low energy sensitization, the following catalytic reductions were carried out under selective lower energy irradiation (>500 nm). Type I and II showed different catalytic performances, primarily due to the choice of solvent for each catalytic condition. A suspension of Type I in 3 mL water containing 0.1 M AscH (pH = 2.66) resulted in efficient photocatalytic hydrogen evolution, producing 37 μmol of H2 for 4 h. However, in photocatalysis of Type II (**SQ**/TiO_2/Re(I)) in 3 mL DMF containing 0.1 M BIH, the TiO_2-bound **SQ** dyes are not capable of working as a low energy sensitizer because **SQ** was susceptible to dye decomposition in nucleophilic DMF condition, resulting in DSC deactivation for the CO_2 reduction. Even with the limitation of solvent, the DSC conditions for utility of **SQ** have been established: anchoring group effect of **SQ** with either phosphonic acid or carboxylic acid onto the TiO_2 surface; energy alignment of **SQ** with the flat band potentials (E_{fb}) of TiO_2 semiconductor and reduction power of electron donor; and wavelength range of the light source used, particularly when >500 nm.

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Spontaneous formation of 3D zinc blende-CdTe by using 2D wurtzite hexagonal CdS template

Seokpyo Jeon, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Ion exchange is a powerful postsynthetic tool for the synthesis of interesting nanoparticle structures. In ion exchange, cation exchange reaction have been studied extensively as the smaller cations can easily diffuse through the anion frameworks of template NPs. In case of anion exchange reaction, however, anions generally diffuse more slowly than cations due to the larger size of anion. Slow anion diffusion often requires longer reaction times and higher temperature than cation exchange. Thorough understanding of anion exchange reaction can expand the range of structure control of ionic NPs. Here we report the synthesis of anisotropic phase-changed 3D zinc blende tetrahedral CdTe NPs via anion exchange of 2D wurzite CdS template. We provide the detailed description of the observed structural evolution as well as the theoretical background for the findings.

Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Elemental segregation in Ir-based nanoframes for efficient water oxidation in acidic media

Songa Choi, Jongsik Park, Kwangyeol Lee[*]

Department of Chemistry, Korea University, Korea

Electrocatalytic oxidation of water have been regarded to play an important role in addressing environmental issues. To date, IrO_x has been the most efficient oxygen evolution reaction (OER) catalyst. However, the IrO_x based nanoparticles can easily dissolve in acidic condition and agglomerate with higher Ohmic resistance to hinder the electronic paths and lower their stability. Therefore, we posited that the integration of Pt/IrO_2 catalysts might be beneficial because the Pt phase can prevent the IrO_x dissolution. Herein, we report a facile synthetic strategy to modulate the degree of interaction of Pt phase with Ir-based nanoframes by controlling the differences in decomposition kinetics and reaction conditions. We also found the optimal degree of interaction between Pt phase and IrO_x phase that shows a greatly enhanced catalytic stability and activity toward OER.

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Poster Presentation : **INOR.P-90**
Inorganic Chemistry
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The binding Constants between Tetrazine Metallamacrocycles with π-Aromatic Guests

YeonJeong Lee, Philjae Kang[1], Younghun Kim[2], Minji Jeong[2], Moon-gun Choi[2,*]

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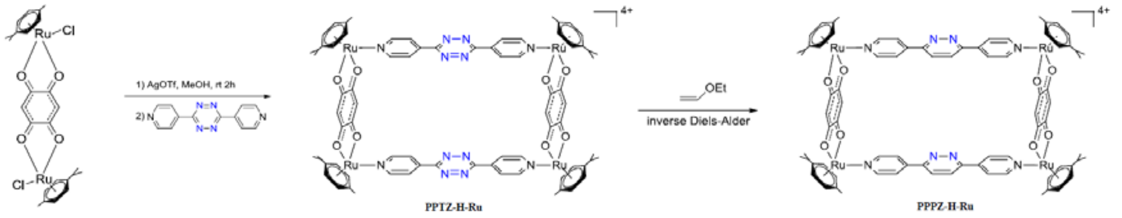
[1]*Department of Chemistry, Hallym University, Korea*
[2]*Department of Chemistry, Yonsei University, Korea*

Metallosupramolecule, which processes well defined pores, has attracted great attention not only because of their elegance architectural beauty but also extraordinal applications in catalyst, gas sorption, storage, and stabilization of labile species. Many efforts to establish synthetic strategies to achieve well-defined metallosupramolecues have been successfully devoted.Tetranuclear ruthenium macrocycles with two 3,6-bipyridyl-*s*-tetrazine ligands were synthesized and their host-guest chemistry with polycyclic aromatic hydrocarbons (PAHs) was investigated. Extremely low π-electron density of the tetrazine rings led the macrocycles to act as efficient receptors of the PAHs via donor-acceptor interactions. Moreover, the *s*-tetrazine moieties of macrocycles were successfully modified to pyridazine, which has relatively rich π-electron density, by inverse electron demanded Diels-Alder reactions. This resulted in dramatic decreases in the binding ability for PAHs.



Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

High catalytic activity of electrochemically activated rhodium phosphosulfide toward hydrogen evolution reaction

Yongju Hong, Haneul Jin, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Developing highly active and robust hydrogen evolution reaction catalysts is of paramount importance for the wide applications of hydrogen energy. Even though various transition metal phosphides, as alternative to Pt-based catalysts, with considerable catalytic performances toward HER have been reported, the pitifully inferior efficiency to that of Pt/C is one of the most crucial issues. As a method to drastically increase catalytic performance, the ensemble effect that is derived from the hetero structures or phases has gained a considerable recent interest. Here, we synthesized rhodium-based heterostructure of phosphides and sulfides through post-phosphorization and found that this additional anion incorporation leads to a great enhancement of catalytic activity of the Rh-based catalyst toward HER.

Poster Presentation : **INOR.P-92**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and structural analysis of unsymetry heteroleptic strontium complexes

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[1]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*
[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Strontium was applied to variety field such as computer memory, superconductors, lectroluminescent films and mixed-electronic ionic conductors for fuel cell electrolytes. All of these application have required the fabrication of strontium containing oxide flims through ALD or CVD. For the deposition of thin films using these techniques, strontium precursors with good stability and volatility are essential. However, storontium has less soluble and poor volume properties, adequate ligand design and synthesis are required. We have studied variety stontium complexes and synthesized by reacting Sr(btsa)2(DME)2 with alkoxide and beta diketonate ligands. Synthesized strontium complexes were fully characterized by single crystal XRD analysis, H - NMR, elemental analysis, and thermal stability was analyzed by TGA. All complexes existed in unsymetric dimer complexes, where strontium metals have five coordination bonds of nitrogen and oxygens.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

[Withdrawal] Transition metal doped copper nitride nanocubes for carbon dioxide reduction reaction

Jinwhan Joo, Chung Man Yu, Kwangyeol Lee[*]

Department of Chemistry, Korea University, Korea

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

An Investigation on Photocatalytic CO_2-to-CO Conversion Activities of Heteroleptic $[Ir(C^\wedge N)_2(N^\wedge N)]^+$-type Complexes-Sensitized TiO_2 Ternary Hybrids ($IrPS/TiO_2/Re(I)$): Immobilization Effect of Ir(III) Photosensitizer on TiO_2 Nanoparticles

Ju Hyoung Jo, Daehan Lee[1], Chul Hoon Kim[2], Sang Ook Kang[2], Ho-Jin Son[2,*]

Korea University, Korea
[1]*Korea University Sejong Campus, Korea*
[2]*Department of Advanced Materials Chemistry, Korea University, Korea*

A series of heteroleptic Ir(III) complexes functionalized with the two phosphonic acid ($–PO_3H_2$) groups ($^{\mathrm{dfppy}}$**IrP**, $^{\mathrm{ppy}}$**IrP**, $^{\mathrm{btp}}$**IrP**, and $^{\mathrm{piq}}$**IrP**) are prepared and anchored onto Re(I) catalyst (ReP)-loaded TiO_2 particles (TiO_2/ReP) to build up a new **IrP**-sensitized TiO_2 photocatalyst system (**IrP**/TiO_2/ReP). The photosensitizing behavior of the **IrP** series was examined in **IrP**/TiO_2/ReP platform for photocatalytic CO_2-to-CO conversion. The four **IrP**-based ternary hybrids showed increased conversion activity and durability than the corresponding homogeneous (**IrP** + ReP) and heterogeneous (**IrP** + TiO_2/ReP) mixed systems. Among the four **IrP**/TiO_2/ReP photocatalysts, the low energy light (>500 nm)-active $^{\mathrm{piq}}$**IrP** immobilized ternary system ($^{\mathrm{piq}}$**IrP**/TiO_2/ReP) exhibited the most durable conversion activity, giving a turnover number of ≥730 for 170 h. A similar kinetic feature in time-resolved photoluminescence measurements of both the $^{\mathrm{btp}}$**IrP**/TiO_2 and TiO_2-free $^{\mathrm{btp}}$**IrP** films suggests that the net electron flow in the ternary hybrid proceeds dominantly via a reductive quenching mechanism, unlike the oxidative quenching route of typical dye/TiO_2-based photolysis.

Poster Presentation : **INOR.P-95**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Enhanced Kinetics and Stability of Water Electrolysis through Synergistic Effects of Cobalt Phosphosulfide

Jinhyoung Jo, Jun Kim, Yongju Hong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

While the continuous consumption of fossil fuels has alarmed the world with innumerable environmental issue, the demand for clean energy sources is expected to rise rapidly in the near future. Water electrolysis has attracted a great attention as the alternative, environment-friendly method for future energy resources, and accordingly, the development of efficient electrocatalysts has become essential. Noble metal-based catalysts including Pt, Ir and Ru are well-known for excellent catalytic performances, however, their low natural abundance and high cost remain to be resolved for use in large scale. Motivated by these problems, the research for earth-abundant materials with both high performance and stability has made a significant progress with meaningful results. Among those recent results, cobalt phosphosulfide (CoPS) has a great potential as the low-cost materials with high catalytic activity toward water electrolysis, however, synthetic strategies to such composition has been limited to substrate-based methods. Herein, we report a colloidal synthesis of Au@CoPS core-shell nanostructure with enhanced catalytic performance. In addition to the mixed composition of P and S, the presence of Au in the catalytic phase induces electronic effects favorable toward water electrolysis.

Poster Presentation : **INOR.P-96**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Green synthesis of silver nanoparticles using plant extract and simple quantification with UV-visible light spectra

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Department of Chemistry, Kyung Hee University, Korea
[1]*chemistry, Daejin University, Korea*
[2]*Department of Chemistry, Daejin University, Korea*

The silver nanoparticles synthesized using plant extracts as reducing and stabilizing agent have been prepared. The effect of the amount of extract, pH and temparature of reaction are investgated.The rate of formation and the amount of synthesized silver nanoparticles were significantly increased with increasing the reaction temperature. Furthermore, the concentration of silver nanoparticles were simply quantified from UV-Vis light spectra. In the current work, experimentally calculated concentration of silver nanoparticles were in good agreement with ICP analyzed amount of silver nanoparticles.

Poster Presentation : **INOR.P-97**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

π-Delocalization Effect of Photosensitizing Heteroleptic Ir$^{\text{III}}$ Complex in Photocatalytic CO_2-to-CO Conversion by Semi-Heterogeneous Hybrid Catalyst (IrPS + TiO_2/Re(I))

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[2]*Korea University Sejong Campus, Korea*

Herein, we report on the synthesis, photophysical/electrochemical properties, and excited-state properties of a series of heteroleptic Ir(III) complexes ([Ir(C^N)$_2$(N^N$^{\text{Aryl}}$)]+, **IrP-Ph**) possessing aryl-extended bipyridyl moiety (C^N = (2-pyridyl)benzo[*b*]thiophen-3-yl (btp); N^N$^{\text{Aryl}}$ = 4,4′-Y_2-bpy (Y = –PhSi(Ph)$_3$) with those of non-extended case for comparison. Their photosensitizing abilities were tested in a homogeneous condition (IrP + ReP) and a mixed heterogeneous photocatalytic system consisting of Ir(III) photosensitizer and Re(I) catalyst (ReP)-immobilized TiO_2 catalytic particles (IrP + TiO_2/Re(I)), where ReP is fac-[Re(4,4′-Y_2-bpy)(CO)$_3$Cl] (Y = $CH_2PO(OH)_2$), and the electron donor (ED) is 1,3-dimethyl-2-phenyl-1,3-dihydrobenzimidazole (BIH). Scheme 1 describes the chemical structures of new phenyl-substituted Ir(III) photosensitizer (**IrP-Ph**) and key components for photolysis with its overall photolysis processes. We found that the π-extension by the introduction of phenyl group effectively improves the overall photocatalytic activity with the stabilization of excited electron by π-delocalization over pyridyl and phenyl rings. This study also presents its structure-activity relationship, providing new insights to the influence of electron delocalization on the excited-state properties of anisotropic Ir(III) photosensitizer.

Poster Presentation : **INOR.P-98**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and Characterization of Cu Precursors for Atomic Layer Deposition of Cu Oxide Thin Films

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[3]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Copper oxide is gaining attention due to favorable interesting characteristics such as environmentally friendly, being cost effective, and having reconfigurable electronic structures. Among many copper oxides, cuprous oxide (Cu_2O) and cupric oxide (CuO) are used in various applications due to their excellent electrical properties. For instance, Cu_2O and CuO show the *p*-type characteristic when they have cubic and monoclinic crystal structures. Such characteristic can be used as gas sensor, anode materials in batteries, thin film transistors (TFTs), solar cells, and photo-catalysts. Generally, chemical vapor deposition (CVD) and atomic layer deposition (ALD) are required to form uniform surface on the substrate. CuO_2 or CuO can be selectively deposited by controlling the oxidation state of the Cu(II) precursors and/or reactant gas. In this study, we synthesized novel Cu(II) complexes as next generation precursors for ALD deposition technique. Synthesized complexes were fully analyzed by various analysis equipments such as infrared spectroscopy (IR), elemental analyses (EA), thermogravimetric analysis (TGA), and single crystal X-ray diffraction. The studies to deposit copper thin films using the copper complex by deposition techniques are ongoing.

Poster Presentation : **INOR.P-99**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Electropolymerized Molecular Chromophore-Catalyst Assemblies for Stable Dye-sensitized Photoelectrosynthesis Cell

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Department of Chemistry and Applied Chemistry, Daegu University, Korea
[1]*Department of Applied Chemistry, Daegu University, Korea*

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

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis of Polymer@MOFs for improved water-resistance

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Metal-organic frameworks (MOFs) usually suffer from hydrolysis, resulting in collapse of porosity and crystallinity. In this poster, we present a facile method for improving water stability of MOFs via protecting metal sites by polymerization.

Poster Presentation : **INOR.P-101**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Reductase components and its electron transfer through

Chungwoon Yoon, Heeseon Yoo, Seung Jae Lee*

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The reduced diferrous state ($Fe^{II}Fe^{II}$) can in turn activate O_2 and initiate a catalytic cycle. MMOB does not have any metal ions and coenzymes; however, this regulatory enzyme acts on the pore region near to the diiron active sites, containing the residues Thr213, Asn214, and Glu240, which are considered key regulators for the electron and/or proton transfer. Catalytic activities are improved in the presence of MMOB and MMOH–MMOB complex, indicating that two MMOB molecules can bind to the hydroxylase component at the diiron active site, regulating methane hydroxylation. The structural information between MMOH and MMOR is required to discover the electron transfer pathway that is crucial for turnover number. Recent studies have proposed that the ferredoxin domain of MMOR shares the binding site with MMOB located in the canyon region of MMOH for electron transfer. In this study, *M. sporium 5* was cultured in a tightly regulated NMS media by supplying methane and air to understand its growth and the expression levels of multi-component enzymes. MMOH was found to be highly expressed in *M. sporium 5*, and it was purified to evaluate its catalytic activities using diverse substrates. MMOB and MMOR were also expressed in *E. coli* via constructed plasmids to obtain highly purified enzymes. The successfully expressed and purified enzymes were utilized to measure specific enzyme activities (SEA), and these results showed that *M. sporium 5* exhibits optimal activity at pH 7.5. The electron transfer environment of MMOR is crucial for the activity of sMMO, and different acidities may change the electron transfer environment. *In vitro* activity measurements demonstrated that alkanes, halogens, benzene, and toluene are oxidized through sMMO, and 2 mol equivalents of MMOB showed optimal activity.

Poster Presentation : **INOR.P-102**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Concanavalin A and structural features through metal coordination

Hara Jang, Seung Jae Lee*

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

The structure and functions of ConA have been intensively studied for its potential contribution to defense mechanisms through interaction with carbohydrates, glycoproteins, metabolites, and signaling molecules from diverse organisms, including microorganisms. Biophysical studies on ConA and pathogen glycoproteins have provided details on their interactions for the field of diagnostic microbiology, and these studies can be extended for detecting and estimating the concentration of viruses. Studies on the structure of ConA from *Canavalia ensiformis*, the jack bean, have demonstrated crucial details, including interaction residues such as hydrogen bonds and salt-bridges with carbohydrates. Reports have shown that heterometal ions, including manganese and calcium ions, are crucial for this interaction with carbohydrates. These metal ions and coordinated residues are located near the loop of carbohydrate interaction residues. Most reported structures were crystallized as complexes, including dimers and tetramers, which could affect the interaction with their binding partners, as sidechains and backbones for sugar binding can be shielded and their orientations may change based on complex formation. The binding affinity of ConA differs based on the buffer conditions, and these differences could be attributed to the formation of different complexes. The structural properties based on specific conditions for crystallization and the binding events of monomers to their binding partners, including microbial pathogens, still need to be elucidated

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Poster Presentation : **INOR.P-103**
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Diiron monooxygenase and substrate hydroxylation through multicomponent enzymes

Jaewoong Park, Heeseon Yoo, Seung Jae Lee*

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

Methane (CH_4) is considered as one of the most important greenhouse gases owing to its 20-fold higher heat capacity compared with that of carbon dioxide (CO_2). Preliminary studies have aimed to elucidate the mechanisms of soluble methane monooxygenase (sMMO) involved in this extremely stable C–H activation (104.9 kcal/mol) through intermediate studies, advanced spectroscopies, and structural researches, mostly in *Methylosinus trichosporium* OB3b and *Methylococcus capsulatus* Bath, although mechanistic studies are still required. To better understand the mechanism of sMMO, we successfully expressed and purified essential components, including MMOH, MMOB, and reductase (MMOR) components from *Methylosinus sporium* 5. MMOH from *M. sporium* 5 was successfully expressed and purified from the native bacteria, and MMOB and MMOR were expressed and purified from *E. coli* using recombinant plasmids. We report the first enzymatic study of highly purified essential components, including MMOH, MMOB, and MMOR. Each component was successfully characterized, and specific enzyme activities were comparable with those of other sMMOs with non-heme diiron active sites. Specific enzyme activity showed that two mole equivalents of MMOB/MMOH demonstrate maximal activity in the presence of substrates and one mole equivalent of MMOR/MMOH is sufficient for this activity. Most substrates showed maximal specific enzyme activities at pH 7.5, and these were confirmed by spectroscopic studies on MMOR and the FAD-domain of MMOR by the subtle changes in the interaction between flavin and MMOR.

Poster Presentation : **INOR.P-104**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Zinc fingers and its structural feature to generate specific interactions with their binding partners

Ka Young Son, Seung Jae Lee*

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Zinc finger proteins are one of the most extensively applied metalloproteins in the field of biotechnology due to their unique structural and functional aspects as transcriptional and translational regulators. The classical zinc fingers are the largest family of zinc proteins, and they play critical roles in physiological systems from prokaryotes to eukaryotes. This presentation provides the structural details of several zinc finger proteins that are present in species ranging from prokaryotes to eukaryotes. The structural comparison of these zinc finger domains provides valuable information to the general authors of *Journal of Microbiology and Biotechnology*. These zinc fingers play pivotal roles because they generate transcriptional and translational activation and suppression against exogenous signals. Classical zinc finger proteins in physiological system play structural roles because they generate a specific fold, the ββα secondary structure, to recognize specific nucleic acids, proteins, lipids, and small molecules. Authors have explained the structural and functional details of zinc finger domains from basic aspects to specific changes. ZIF268, TFIIIA, GAGA, and Ros belong to the classical zinc finger family.

Poster Presentation : **INOR.P-105**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis of Highly Bright Green Zn-Ag-In-S/Zn-In-S/ZnS Quantum Dots for White Down-Converted LEDs with a High CRI

Minji Ko, Seoyeon Shin, Hyeongjin Lee[1], Young rag Do[2,*]

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We synthesized highly bright green Zn-Ag-In-S/Zn-In-S/ZnS (ZAIS/ZIS/ZnS) quantum dots (QDs) to realize white down-converted light-emitting diodes (DC-LEDs) with a high color rendering index (CRI, R_a). To enhance the photoluminescence quantum yield (PLQY), we used a high concentration of zinc acetate dihydrate, which is capable of causing the formation of a Zn-In-S inner-shell. The obtained ZAIS/ZIS/ZnS showed a high PLQY of 0.84 with a peak wavelength of 511 nm. We also confirmed the formation of Zn-In-S via X-ray diffractometry and Raman spectroscopy. Furthermore, we fabricated synthesized green ZAIS/ZIS/ZnS , red ZCIS/ZnS QDs, and a cup-type blue InGaN LED to realize multi-packaged white down-converted LEDs with a high CRI. The multi-packaged white DC-LEDs exhibit a high luminous efficacy (LE) value of 76 lm/W at an applied current of 180 mA and a CRI of 91.

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Single crystal to single crystal transformation of non-interpenetrated metal-organic frameworks to doubly interpenetrated metal-organic frameworks with topology conversion

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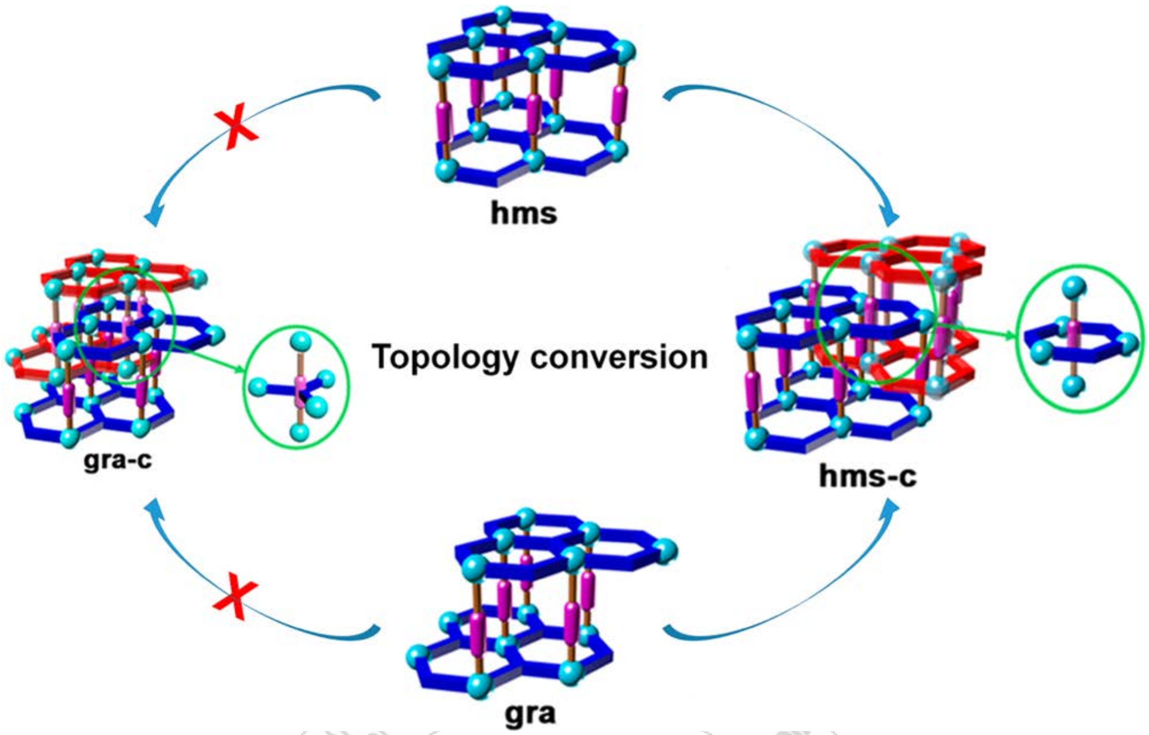
Non-interpenetrated 3D metal-organic frameworks (MOFs) with both an interpenetration-favorable (3,5)-c hms topology and an interpenetration-unfavorable (3,5)-c gra topology are converted to doubly interpenetrated analogues with hms-c topology by thermal treatment, even in the absence of solvent. Depending on conversion temperature and the properties of the pillaring ligand in the non-interpenetrated 3D MOF, which is based on 2D sheets with 3-c hcb topology pillared by neutral ditopic linkers, the pillaring ligands in the interpenetrated MOFs produced are partially removed during the thermal conversions, leading to interpenetrated MOFs that simultaneously contain both micro- and mesopores.


hms
gra-c
Topology conversion
hms-c
gra

Poster Presentation : **INOR.P-107**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Elucidation of defensive mechanisms of halophytes through ROS regulation by indole derivatives

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

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 report, *S. glauca* 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.

Poster Presentation : **INOR.P-108**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Lectins and its carbohydrate binding through heterometal coordinated interactions

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Concanavalin A (ConA) interacts with carbohydrates as a lectin, and recent reports proposed its application for detecting a diversity of viruses and pathogens. Structural studies have detailed the interaction between ConA and carbohydrates and the metal coordination environment with manganese and calcium ions (Mn-Ca-ConA). In this study, ConA was crystallized with a cadmium-containing precipitant, and the refined structure indicates that Mn was replaced by Cd (Cd-Ca-ConA). The structural comparison with ConA demonstrates that the metal-coordinated residues of Cd-Ca-ConA, that is Glu8, Asp10, Asn14, Asp19, and His24, do not have conformational shifts, but residues for sugar binding, including Arg228, Tyr100, and Leu99, reorient their side chains, slightly. Previous studies demonstrated that excess cadmium ions can coordinate with other residues, including Glu87 and Glu183, which were not coordinated with Cd in this study. The trimeric ConA in this study coordinated Cd with other residues, including Asp80 and Asp82, for complex generation. The monomer does not have specific interaction near interface regions with the other monomer, but secondary cadmium coordinated with two aspartates (Asp80 and Asp82) from monomer 1 and one aspartate (Asp16) from monomer 2. This study demonstrated that complex generation was induced via coordination with secondary Cd and showed the application potential regarding the design of complex formation for specific interactions with target saccharides.

Poster Presentation : **INOR.P-109**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication of a Red, Green and Blue Integrated Copper Indium Gallium Sulfide Selenide Solar Cell with a Narrow-Bandwidth Stop Filter

Gang Yeol Yoo, SeungJe Lee[1], Woong Kim[2,*], Young rag Do[3,*]

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[3]*Department of Bionano Chemistry, Kookmin University, Korea*

We introduced pure red, green and blue (RGB) color-generated copper indium gallium sulfide selenide (CIGSSe) solar cells with a narrow-bandwidth stop filter (NBSF) created through an adaptation of a screen printing method. High-purity RGB color was generated by an interference effect with a high refractive index and a low refractive index in an alternating approach. To eliminate the air gap between the surface of CIGSSe solar cell and the glass substrate of the NBSF, screen printing and a low-temperature annealing process with polydimethylsiloxane (PDMS) was introduced. The thickness of the passivated PDMS glue used was 50 µm. The optical properties of the integrated RGB color-generated CIGSSe solar cell were examined by means of reflectance spectroscopy and from images taken by a digital camera. The performance capabilities of the RGB-integrated CIGSSe solar cells were assessed using J-V measurements under AM 1.5G (100 mW cm^{-2}) and by external quantum efficiency (EQE) measurements.

Poster Presentation : **INOR.P-110**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Luminescence Differences in InGaN/GaN Blue LEDs According to the Electrode and ITO Shape

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[3]*Division of Advanced Materials Engineering, Korea University, Korea*
[4]*Department of Bionano Chemistry, Kookmin University, Korea*

With the development of GaN-based optoelectronic devices, the need for p-GaN contacts with low resistivity, good thermal stability, and high transparency or reflectivity has become more pressing. In this study, InGaN/GaN blue LEDs 750 × 750 μm^2 in size with an indium tin oxide (ITO) layer emitting at 450 nm were fabricated. A vacuum evaporation technique was utilized to deposit ITO on p-GaN with a thickness of 150 nm as a spreading layer. When an ITO was etched, a mask was created using a positive photoresist (PR) with a contact aligner and etched by a copper etchant. One problem with chemical etching is that the shape that is etched depends on the temperature and the etching time. The best etching shape is similar to the L-shape of GaN, though somewhat smaller. To solve this problem, we studied how to change the pad shape to compensate for the problems created by ITO etching. Previously, square pads were created in n-GaN and p-GaN, but the complement was to make the full contact by attaching wings to the p-pad part. Each procedure was confirmed by an optical microscope, and the efficiency was measured by a probe station.

Poster Presentation : **INOR.P-111**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Stable $CsPbX_3/CsPb_2br_5$ Core/Shell Perovskite Nanocubes for Wide-Color-Gamut LCDs

Hyeongjin Lee, Minji Ko, Young rag Do*

Department of Applied Chemistry, Kookmin University, Korea

Quantum dots (QDs) are promising materials for displays due to their good photoluminescent properties, such as their high photo-luminescent quantum yield (PLQY) and easy color tunability. Specifically, perovskite nanocubes are most promising because they have very narrow full-width-at-half-maximum (FWHM), a very high PLQY, and easy color tunability. They are also easy to synthesize. However, perovskite nanocubes are associated with problems related to their stability depending on UV exposure and on the humidity and temperature. If we solve these problems, perovskite nanocubes can be used for very wide-color-gamut liquid crystal displays (LCDs). Here, we synthesized stable $CsPbX_3/CsPb_2br_5$ core/shell perovskite nanocubes and fabricated wide-color-gamut LCDs. The PLQYs of the green (G) and red (R) core/shell perovskite nanocubes synthesized in this study are ~77.4% and ~78.9%, respectively. The enhanced stability of the perovskite nanocubes against certain UV, humidity and heat conditions allows perovskite nanocube film to be applied to color-converting materials of LCDs. The conversion efficiency rates of a perovskite-nanocube emissive LCD consisting of G and R perovskite nanocube films sandwiched in the form of a recycling bottom layer and a blue-filtering top dichroic filter are 42.0% and 44.3%, respectively. The color gamut was enlarged to 134% compared to the NTSC standard. The GR colloidal perovskite nanocubes and the fabricated perovskite nanocube films were analyzed by TEM, XRD, and EDX in terms of their structural properties and by PL and EL with an integrating sphere with regard to their optical properties.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Three-Package White LED Backlighting Applications Using Narrow-Band $SrMgAl_{10}O_{17}$:Eu,Mn Green Phosphors and Photoluminescence Properties

Heejoon Kang, Keyong Nam Lee[1], Young rag Do*

Department of Bionano Chemistry, Kookmin University, Korea

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

$BaMgAl_{10}O_{17}$ (BAM) phosphors have long been used for plasma display panels (PDPs) due to the good quality of their blue emission. However, due to their use of the harmful vacuum ultraviolet (VUV) wavelength range, they are no longer used. In this study, the cation was changed to the Sr^{2+} ion using a BAM phosphor and the excitation light was enhanced in addition to the red shift of the excitation spectrum through Eu^{2+} and Mn^{2+} co-doped SAM phosphors, allowing the use of a near-blue LED. The PL emission spectrum of the optimized SAM:Eu,Mn phosphor peaks at 518 nm at a full-width-at-half-maximum (FWHM) of 26 nm under LED excitation at 432 nm. Through this result, we fabricated three-package down-converted white-LEDs (DC-WLEDs) with a 432 nm blue LED and $K_2SiF_6:Mn^{4+}$ (KSF:Mn) red phosphors. The color gamut area of a color-filtered RGB triangle of DC-WLEDs incorporated with the optimum SAM:Eu,Mn green and KSF:Mn red phosphors is enlarged by 114% relative to that of the NTSC standard system in the CIE 1931 color space. The luminous efficacy of our DC-WLED was measured and found to exceed 90 lm/W at 20 mA.

Poster Presentation : **INOR.P-113**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Analysis of the Visual and Nonvisual Properties of a CCT-Tunable White LED on Human Retinal Photoreceptors

Yun Jae Eo, Keyong Nam Lee, Young rag Do*

Department of Applied Chemistry, Kookmin University, Korea

The advent of artificial lighting source, such as incandescent bulbs, fluorescent tubes and light-emitting diodes (LEDs), has changed our lives dramatically. In recent years, the efficiency of these types of lighting, i.e., the visual properties, and the effects of artificial lighting on humans, such as their nonvisual properties, have become increasingly important. Lately, the spectral functions, quantities and metrics pertaining to retinal photoreceptors were defined as an international standard. In particular, intrinsically photosensitive retinal ganglion cells (ipRGCs), which contain the photopigment melanopsin, are known as a type of photoreceptor that exhibits nonvisual properties by means of incident light. In this study, we fabricated phosphor-converted LEDs (pc-LEDs) in order to realize a white indoor lighting that offers varying correlated-color temperatures (CCTs). Tetra-chromatic (red, amber, green and blue) multi-packaged white LEDs were able to achieve white light with a CCT from 2,000 K to 10,000 K. In addition, implementable white spectral power distributions (SPDs) were obtained using an illuminance spectrophotometer, and we analyzed the visual and nonvisual properties with the spectral sensitivity functions of the photoreceptors.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Fabrication of a Moth-Eye Structure via Polystyrene Nanosphere Lithography to Reduce Reflective Losses

SeungJe Lee, Gang Yeol Yoo[1], Woong Kim[2], Young rag Do[3,*]

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[2]*Division of Advanced Materials Engineering, Korea University, Korea*
[3]*Department of Bionano Chemistry, Kookmin University, Korea*

Moth-eye structures offer the advantage of reducing reflective losses. Instead of the traditional polydimethylsiloxane (PDMS) stamping method, we fabricated such a structure on a glass substrate via a nano-sphere consisting of a hexagonal-closed-packing array in an attempt to improve the light extraction efficiency. These moth-eye structure patterns were fabricated by a combination of polystyrene (PS)-based nano-sphere lithography (NSL) and reactive ion etching (RIE). We confirmed the functionality of the moth-eye structure for use given their anti-fogging effect. The moth-eye structure was also investigated using a scanning electron microscope (SEM). The scattering effects of the nanostructure were measured by UV-vis spectroscopy and by reflectance measurements.

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Size and Thickness Effects of Surface Passivation on an ITO-Insulator-Metal Structure with Atomic-Layer-Deposited Al_2O_3

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Kookmin University, Korea
[1]*Department of Bionano Chemistry, Kookmin University, Korea*

Stacked ITO-insulator-metal (Ti) structures with atomic-layer-deposited Al_2O_3 were fabricated to suppress the reverse leakage current and improve the breakdown voltage. The effects of Al_2O_3 surface passivation based on the size and thickness of the ITO-Al_2O_3-Ti overlapping area were studied through current-voltage measurements. Stacked structures with Al_2O_3 thicknesses of 40 nm, 80 nm, and 100 nm fabricated by atomic layer deposition (ALD) showed direct proportional relationships between the corresponding breakdown voltage points. In addition, an inverse proportional relationship between the size of the overlapping area and the breakdown voltage point was experimentally determined. The findings of this study suggest that an appropriate size and thickness of Al_2O_3 in ITO-insulator-metal structures can improve the breakdown voltage and decrease the reverse leakage current.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and Structural Characterization of [(L_{DTEDA})MBr_2] (M = Co, Zn, Cd) for Ring Opening Polymerization of *rac*-Lactide

Kyeonghun Kim, **Hyosun Lee***

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of cobalt(II), cadmium(II) and zinc(II) complexes, **[(L_{DTEDA})MBr_2]**, supported by ligand (E)-N^1,N^1-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine **(L_{DTEDA})**. All complexes were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, elemental analyzer and single crystal X-ray diffraction. Specifically, molecular structure of **[(L_{DTEDA})$CoBr_2$]** exhibited distorted tetrahedral geometry around cobalt metal center. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of MeLi were investigated at 25℃.

Poster Presentation : **INOR.P-117**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Carbon Nano-Onion-Based Twin mode ‘Turn-On/Off’ Sensor Array for Perilous Organic Solvents

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Nanochemistry, Gachon University Global Campus, Korea
[1]*Department of Chemistry, Kunsan National University, Korea*
[2]*Department of Chemistry, Kyungpook National University, Korea*

Nowadays, the sensing of volatile organic solvents (VOCs) is very crucial for monitoring air quality, water safety, and other environmental applications. Conventionally, various analytical techniques including gas chromatography, mass spectrometry, high-pressure liquid chromatography have been reported to detect VOCs, although most of the techniques are highly time-consuming and expensive. Here, we reported a novel and cost-effective strategy for the green synthesis of carbon nano onion (CNOs) from the waste part (endocarp) of mango seed, and we used as an electrode material as well as fluorescent material for the sensing of highly toxic volatile organic solvents (VOCs). The carbon nano onion (CNOs) were prepared by a simple solvent-free hydrothermal method at the temperature of 170 °C. The synthesized CNOs showed blue fluorescent and were in a size range of 25 – 32 nm with interlayer spacing 0.27 nm. The designed sensor exhibits highly efficient and rapid dual-mode ('turn on' and 'turn off') fluorescent detection as well as electrochemical detection of DIPA and dioxane. Markedly, this ultra-low sensing achieved from the hydrogen bonding between the surface functional group in CNOs and hosted amine and dioxane. This observation supported by the visual detection of DIPA in an aqueous medium. The calculated limit of detection (LOD) for DIPA was in ultra-low level (0.369 pM). Besides, the electrochemical oxidation of DIPA involves the transfer of an electron from amine to the CNOs modified electrode-electrolyte interface. The sensitivity of DIPA in electrochemical sensing found to be 2.35 nM. Credibly, DIPA, and dioxane considered as a toxic chemical and detected with high sensitivity, portraying this CNOs as a potential sensor for environmental application.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **INOR.P-118**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Adsorption of silicon tetrahalides for atomic layer deposition of silicon nitride: a theoretical study

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Department of Chemical Engineering, Hongik University, Korea

Atomic layer deposition (ALD) is a promising technique for deposition of the ultra-thin films with atomic scale precision. To better understand the mechanism by which ALD occurs, we simulated the chemical adsorption reaction of silicon tetrahalide precursors (SiCl4, SiBr4, and SiI4) on the NH2-terminated silicon cluster using density functional theory (DFT). All silicon tetrahalides chemisorb on the surface via sequential formation of Si-N bonds and releasing hydrogen halide as gaseous byproduct. The enthalpy of reaction shows a periodic trend in the order of SiCl4, SiBr4, SiI4, such that the reactions of SiI4 are less endothermic in general. As more ligands are removed from the precursors, the reaction becomes more endothermic, and the activation energy of the reactions increases. For some silicon tetrahalide precursors, the critical transition states involve change of the molecular geometry, while some transition states are those of Si-X bond dissociation. Our results have implications for assessment of the temperature window of silicon nitride ALD using various precursors.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Non-Planarity in 2D porphyrinic Metal-Organic Frameworks

Junghye Lee, Eunji Jin, Wonyoung Choe*

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

Porphyrin containing proteins such as heme, cytochromes, and chlorophyll have been studied for their interesting biological functions such as oxygen transport, storage, and electron transfer. According to recent studies, porphyrin distortions (non-planar porphyrins) play a key role in the controls the functions such as redox potential, and binding affinity. There have been many studies on the relationship between non-planar porphyrins and biofunctions on the supramolecular chemistry. However, numerous researches have been done with non-planar porphyrin molecules on the molecular level, the field of porous materials is still its infancy.In this work, we successfully obtained new 2D porphyrinic MOF, UPF-100 (UPF represents UNIST porphyrin framework) constructed with elongated non-planar porphyrin ligand and copper paddle wheel. UPF-100 show unique structural characteristics such as waved layer sheets and zig-zag pore channels. In addition, we synthesized UPF-100 nanosheets via surfactant-mediated protocols. We show that UPF-100 can the impact fundamental research as well as energy applications.

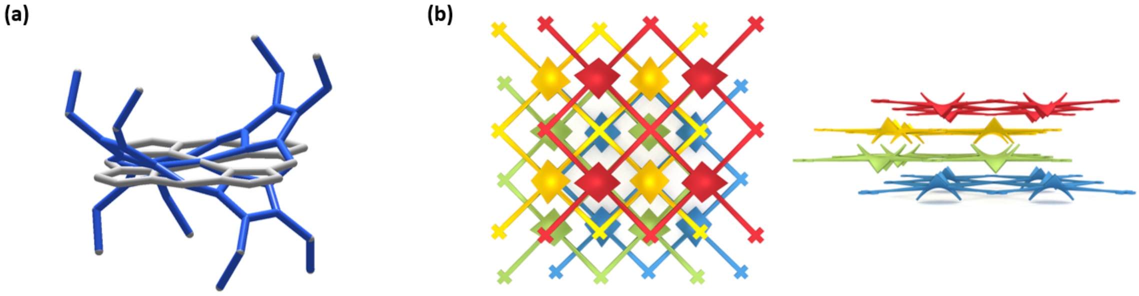


Figure 1. (a) Overlay of planar porphyrin ring (grey) and saddle-distorted porphyrin ring (blue). (b) The top view and side view of UPF-100 structure.

Poster Presentation : **INOR.P-120**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

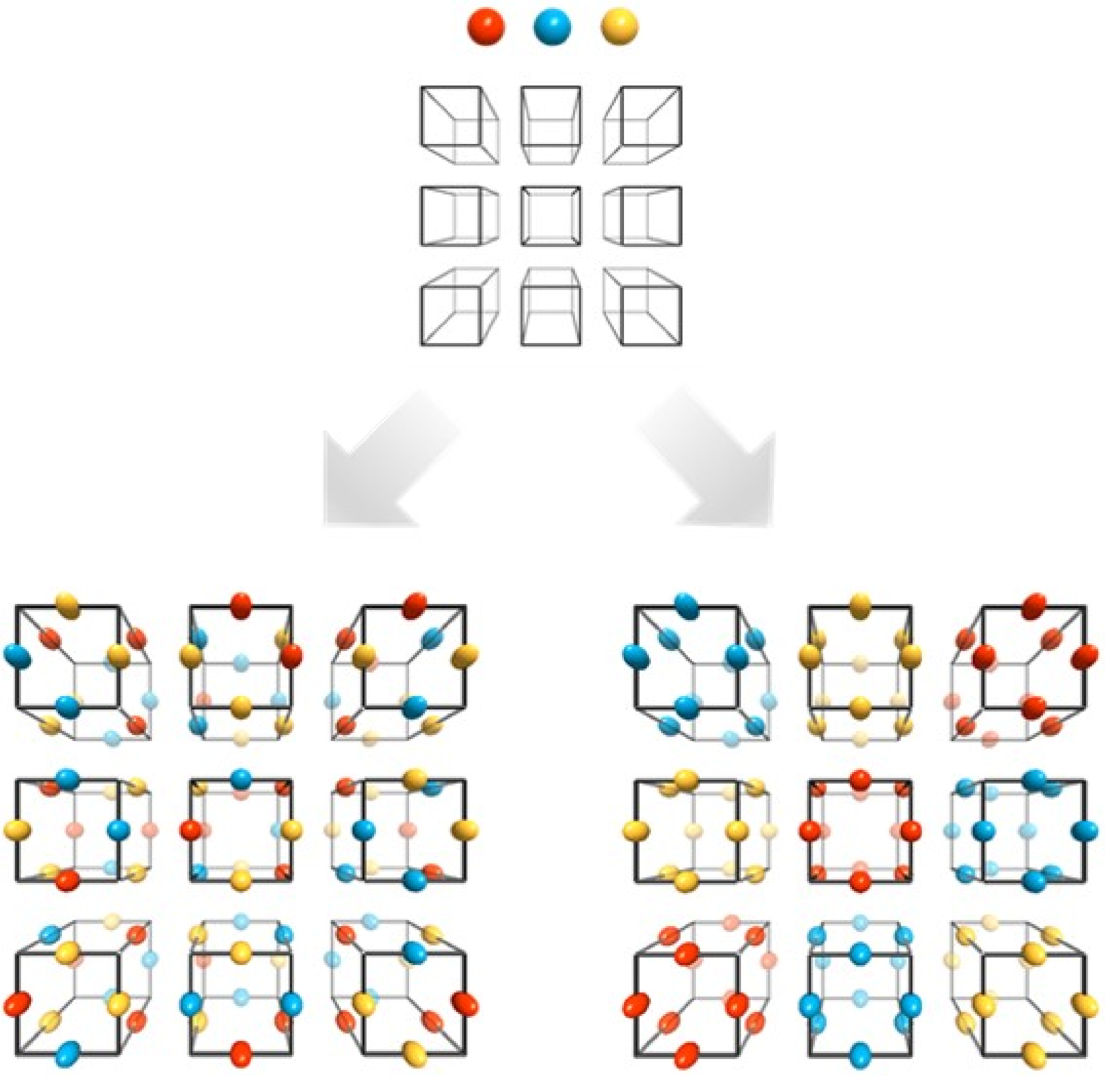
Isoreticular Zr-Based Metal-Organic Polyhedra as Multivariate Porous Platforms

Dongsik Nam, Jiyeon Kim, Wonyoung Choe*

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

Chemical and physical properties of porous solids are closely related to interactions between frameworks and guests in pores. The chemical environment of pores is highly tunable especially in metal-organic frameworks (MOFs). Thanks to rational structural design and rich choices of molecular building blocks, MOFs can accommodate multiple functional groups while the frameworks retain the backbone structures. Although the multivariate MOFs with various functionalized linkers showed novel properties, there is a still daunting challenge in understanding how diverse pore types are formed and controlling the pore population. In this poster presentation, we demonstrate, as an advanced multivariate platform, an isoreticular series of Zr-based metal-organic polyhedra (MOPs) with various combinations of functionalities (-H, -CH3, -NH2, -OH, -(CH3)2, -Br). A new synthetic method includes a mixed-cage strategy where the functionalized cages are mixed, compared with a mixed-linker strategy which yields a random distribution of functionalities (Figure). The clear differences in the cage population between mixed-linker and mixed-cage systems were observed in the mass spectra when the complexity increased from binary to senary mixing systems. This study highlights the potential of isoreticular MOPs for multiple functionalization and control of the component population, suggesting a new platform for emerging properties in multivariate porous solids.

Metal-organic polyhedra



Poster Presentation : **INOR.P-121**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Decomposition of dimethylmethylphosphonate (DMMP) with UV-C radiation

Jongho Yoon, Etae Choi, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Due to a tremendous threat of terrorism with chemical warfare agents (CWAs) including Tabun (GA), Sarin (GB), Soman (GD) and VX, the decomposition of CWAs has received much attention for decades. CWAs are tremendously lethal chemicals that can be used as a gas, liquid, aerosol and/or powder. Although there are hundreds of known-toxic materials, only some of them are treated as CWAs. These materials are well-proven to show lethal and incapacitating effects to human. Therefore, the decomposition or detoxification of CWAs is one of the most important issues in national security and public safety. In the present time, photocatalytic reaction of phosphonates is one of the most widely used methods for CWA decomposition. They are often composed of hybrid systems containing TiO_2 or ZnO photocatalyst and often show great performance for the degradation of CWAs such as soman, sarin and VX. However, they are usually encountered a great limitation in practical use, and it is highly demanded that a system can be easily used in the field.In this presentation, we like to demonstrate an effect of UV-C radiation for the decomposition of DMMP which is one of the most widely used chemical simulants. This result would show a great impact in the fabrication of personal detoxification device that can be used in the field and play an important role for national security and public safety.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and Characterization of Transition Metal Complexes of Bis(thiosemicarbazone) Ligand

Haewon Jeong, Hyeri Jeon, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea

.Thiosemicarbazones and their metal complexes have attracted much attention due to their potential donor atoms (e.g., nitrogen and sulfur) and configurational flexibility; they have presented versatile utilities in a broad field of biology, pharmacology, supramolecular chemistry and energy production processes. In this work, bis(thiosemicarbazone) ligand derivatives were synthesized with transition metals [Fe(II), Co(II), Ni(II), Cu(II), Zn(II)]. The synthesized complexes were characterized by using: UV-visible spectroscopy, electrospray ionization mass spectrometry (ESI MS), and X-ray crystallography.

Poster Presentation : **INOR.P-123**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and Chacterization of First-Row Transition Metal Complexes with Bis(semicarbazone) Ligand

Hyeri Jeon, Haewon Jeong, Seungwoo Hong[*]

Department of Chemistry, Sookmyung Women's University, Korea

Semicarbazones have been attracted much attention due to its extensive presence in natural products, pharmaceutical compounds and synthetic polymers. A series of coordination complexes of first-row transition metals bearing bis(semicarbazone) ligand, [M(dapsc)] (M = Mn(II), Fe(II), Co(II), Ni(II), Cu(II) and Zn(II); dapsc = (2E,2'E)-2,2'-(1,1'-(pyridine-2,6-diyl)bis(ethan-1-yl-1-ylidene))bis(hydrazinecarboxamide)) have been synthesized. The metal complexes have been characterized by using various spectroscopic methods such as UV-vis spectroscopy, electrospray ionization mass spectrometry (ESI MS), and X-ray crystallography. X-ray crystal structures of the metal complexes bearing dapsc ligand show that the (Mn(II), Fe(II), Co(II), Ni(II), Zn(II)) complexes are seven-coordinated pentagonal-bipyramidal geometry whereas the Cu(II) complex is six-coordinated distorted octahedral geometry.

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

Investigation of the Driving Force for the Phase-Transition in the $\mathrm{Ca}_{2-x}RE_x\mathrm{CdSb}_2$ (M = Yb, Eu; $0.11(1) \leq x \leq 1.36(2)$) System

Ki Won Kim, **Tae-Soo You**[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Total nine of the quaternary Zintl compounds belonging to the $\mathrm{Ca}_{2-x}RE_x\mathrm{CdSb}_2$ (RE = Yb, Eu; $0.11(1) \leq x \leq 1.36(2)$) system have been synthesized by the Pb metal-flux method and characterized by powder and single crystal X-ray diffractions analyses. The title compounds show two similar but slightly different crystal structures, which are the $\mathrm{Ca_2CdSb_2}$- and $\mathrm{Yb_2CdSb_2}$-type. In particular, we observed the phase transition from the $\mathrm{Ca_2CdSb_2}$- to $\mathrm{Yb_2CdSb_2}$-type depending upon an amount or a type of substituents in the title system. In addition, during the investigation, we observed a particular cationic site-preference over two available sites. To understand the driving force for this phase-transition and the cationic site preference, a series of the TB-LMTO calculations was conducted, and the resultant DOS, COHP, and ELF were thoroughly interrogated. According to COHP analyses, the observed phase-transition is triggered by the energetically unfavorable cation interactions in the Yb-rich $\mathrm{Ca_2CdSb_2}$-type phase, and the site-preference can be explained by the QVAL of the particular cationic sites based on the electronegativity of each atomic site.

Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Exhibition Hall 1, THU 11:00~12:30

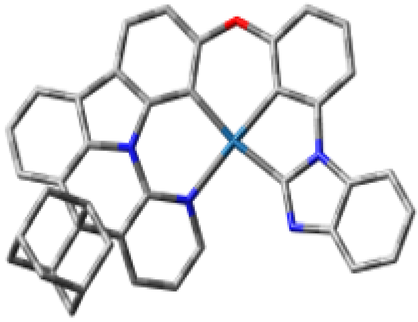
DFT/TD-DFT study on the a symmetric cyclo-metalated platinum (II) complexes with tetra-dentate ligands: Structural feature and photo-chemical properties

Hojune Choi, Soon-Ki Kwon[1,*], Bong Gon Kim[*]

Department of Chemical Education, Gyeongsang National University, Korea

[1]*Department of Materials Engineering and Convergence Technology and ERI, Gyeongsang National University, Korea*

In this study, DFT(density functional theory) and TD-TDFT(time-dependent functional theory) calculations were employed to investigate the geometries, electronic structures, reorganization energy and photo-chemical properties of six cyclometalated Pt(II) complexes with tetra-dentate asymmetric ligands. The platinum complexes have the general structure [Pt(CzPy^O^ppz)] and [Pt(CzPy^O^pIz)], where a tetradentate cyclometalating ligand is consisting of CzPy (carbazolylpyridine), ppz (3,5-dimethyl-1-phenyl-pyrazole), pIz(3-methyl-1-phenyl-imidazole) components, and an oxygen bridging group. And Pt(II) complexes with several tetra-dentate ligands derivative form linked cyclohexyl and adamantly substituents. The geometric structures of the complexes in the ground and excited states were explored at the B3LYP and UB3LYP levels, respectively. The absorption and emission spectra of the complexes in CH_2Cl_2 solutions were calculated by time-dependent density functional theory (TD-DFT) with the PCM solvent model. According to the results, Electrochemical analysis indicates that reduction process occurs mainly on the electron-accepting pyridyl group, and the irreversible oxidation process is primarily localized on the metal-phenyl portions. The studies of their photo-physical properties indicate that the lowest excited state of the platinum complexes is a ligand-centered $3\pi-\pi^*$ state with minor to significant 1MLCT/3MLCT character and are strongly dependent on the nature of the electron accepting pyridyl moiety.



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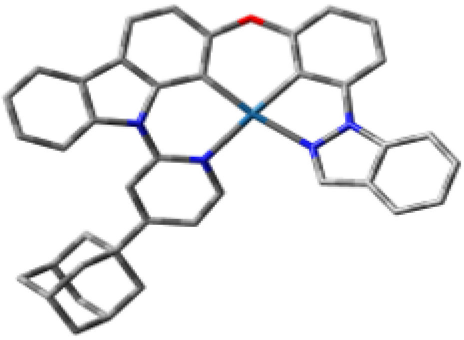


2

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

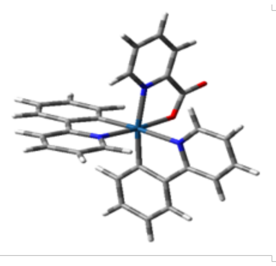
Exhibition Hall 1, THU 11:00~12:30

DFT/TD-DFT Study on the Geometric preference and Photo-chemical properties of Ir(PPy)$_2$(L), L=PPy, Pic, bpy and acac

Dong-Seon Shin, Hojune Choi, Yun Hi Kim[1,*], Bong Gon Kim[*]

Department of Chemical Education, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

Recently, Ir(PPy)$_3$ is very attractive interested in research items for organic lighted emission diodes fields. And Ir(PPy)$_2$(L), L is ancillary ligands as pic and bpy, are also many interested in complexes. These Ir(A-B)$_3$ type octahedral complexes are consist on various geometrical isomer according to ancillary ligands. Ir(PPh)$_3$ complexes presents two different geometrical isomers as facial and meridional, Ir(PPy)$_2$(Pic) are presented four different geometrical isomers. In this study, four different octahedral Ir(III) complexes, Ir(PPy)$_2$(L), L are ppy, bpy, acac and pic as ancillary ligands to identify geometrical preference and emission patterns. This includes structural properties, spectral properties, molecular orbital (MO) descriptions, and ionization energies. The latter is germane to OLED devices because the ionization energies and electron affinities (commonly referred to as the HOMO and LUMO energies, respectively) of the light-emitting molecules in the active layer need to be matched to the energy levels of the electrodes.According to results, The fac-Ir(ppy)$_3$ having the lower energy. Because fac-Ir(ppy)$_3$dominates in most environments, focus is on this species. Time-dependent density functional theory using B3LYP functional is used to calculate excited states of Ir(ppy)$_3$ and a few low energy states of Ir(ppy)$_3$. The calculated T_1 –S_0 energy gap (2.30 eV) is in reasonable agreement with the experimental value of 2.44 eV. Equilibrium geometries are calculated for S_0, T_1, and the lowest cation state (D_0), and several ionization energies are obtained: adiabatic (5.86 eV); vertical from the S_0 equilibrium geometry (5.88 eV); and vertical ionization of T1 at its equilibrium geometry (5.87 eV). These agree with a calculation by Hay (5.94 eV), and with the conservative experimental upper bound of 6.4 eV. Molecular orbitals provide qualitative explanations. A calculated UV absorption spectrum, in which transitions are vertical from the S_0 equilibrium geometry, agrees with the room temperature experimental spectrum. The calculated T_1 –S_0 energy gap (2.30 eV) is in reasonable agreement with the experimental value of 2.44 eV. Only a few percent of singlet character in T_1 is needed to explain so short a phosphorescence lifetime as 200 ns, because of the large $^1\mathrm{LC} \leftarrow S_0$ and $^1\mathrm{MLCT} \leftarrow S_0$ absorption cross-sections. Equilibrium geometries are calculated for S_0, T_1, and the lowest cation state, and several ionization energies are obtained: adiabatic (5.86 eV); vertical from the S_0 equilibrium geometry (5.88 eV); and vertical ionization of T_1 at its equilibrium geometry (5.87 eV).



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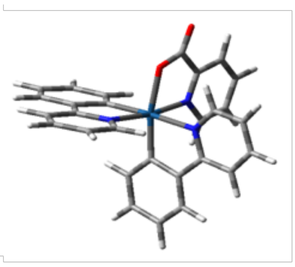

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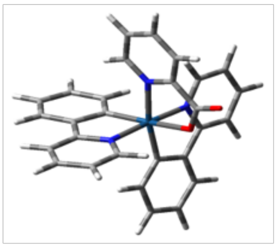

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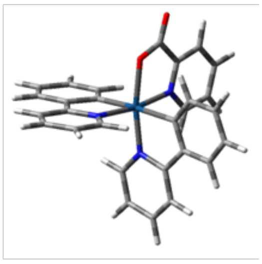


4

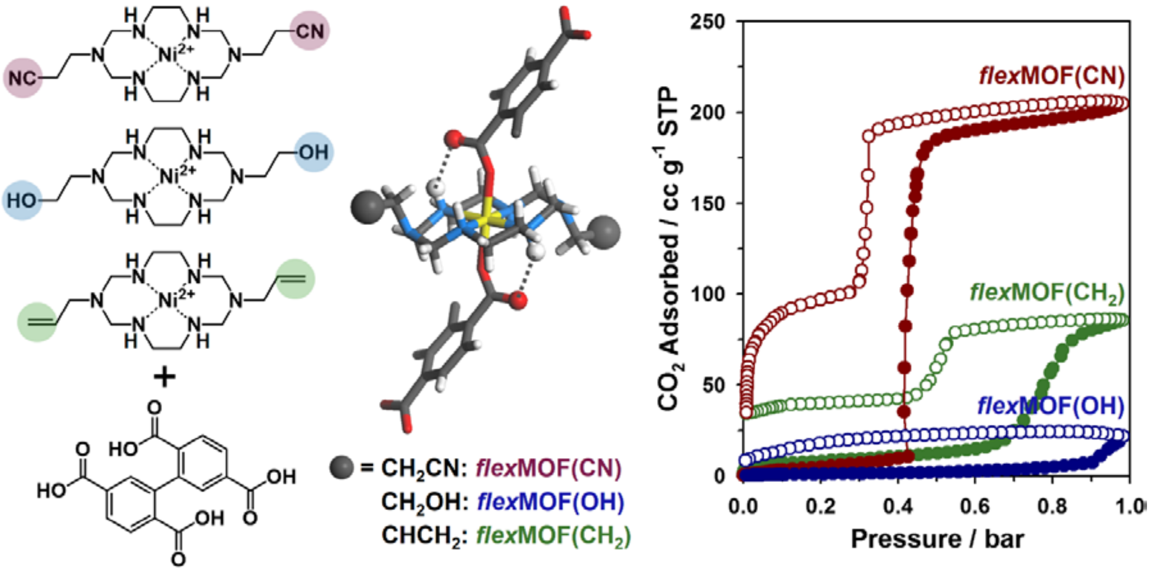
Poster Presentation : **INOR.P-127**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Tuning of the flexibility in metal-organic frameworks based on pendant arm macrocycles

<u>Sungeun Jeoung</u>, Jaehwa Lee[1], Soochan Lee[1], Wonyoung Choe[1], Dohyun Moon[2,*], Hoi Ri Moon[1,*]

Department of chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*
[2]*Beam Operation Team, Pohang Accelerator Laboratory, Korea*

An isostructural series of flexible metal-organic frameworks based on macrocycles having diverse pendant arms was developed to tune flexibility depending on functional groups. The pendant arms directing into the pores were found to play a key role in imparting different gate-opening behaviors in the threshold pressure and sorption capacity upon interaction with guest molecules.



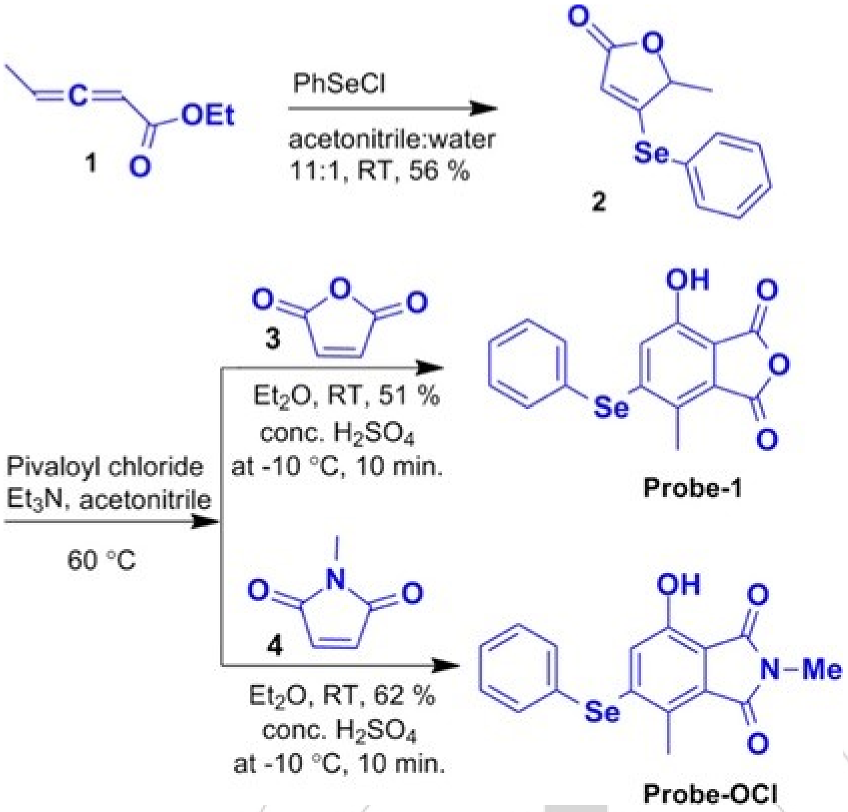
Poster Presentation : **INOR.P-128**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

Selenium-based ROS Biological Probes: Mycophenolic acid Core Intermediates as a New Chemosensing Fluorophore Class

David George Churchill

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

Herein, we have designed, synthesized, and characterized novel compounds. We have been interested in targeting organoselenium-based molecules (Probe-1 and Probe-OCl) based on a synthetic intermediate of mycophenolic acid (MPA) for the aqueous detection of OCl^-. Hypochlorous (OCl^-) ion is the most well-known bacterial oxidant; it is produced by neutrophils. Excess amounts of OCl^- are known to cause various disorders in living systems. Both molecular probes show immediate “turn on” fluorescence upon the addition of OCl^-; they display an increase in the fluorescence quantum yield (3.7-fold for Probe-1 and 11.6-fold for Probe-OCl) and are completely soluble in aqueous media without the help of cosolvent (see figure below). However, a decrease in “turn-on” intensity with the oxidized version (-Se(O)-) of Probe-1 in cell assays due to the anhydride/phthalate functional group suggests probe degradation is occurring based on the hydrolytic action (probe degradation half-life = ~1500 seconds at 15 μM of Probe-1 and 150 μM OCl). Thus, the change of “anhydride” to “methylamide” affords Probe-OCl more stability without sacrificing its water solubility properties. We are derivatizing further to expand the practicality of this fluorophore class.


OEt
O
1
PhSeCl
acetonitrile:water
11:1, RT, 56 %
O
O
Se
2
O
O
O
3
Et$_2$O, RT, 51 %
conc. H$_2$SO$_4$
at -10 °C, 10 min.
OH
O
O
O
Se
Probe-1
Pivaloyl chloride
Et$_3$N, acetonitrile
60 °C
O
N
O
4
Et$_2$O, RT, 62 %
conc. H$_2$SO$_4$
at -10 °C, 10 min.
OH
O
N–Me
O
Se
Probe-OCl

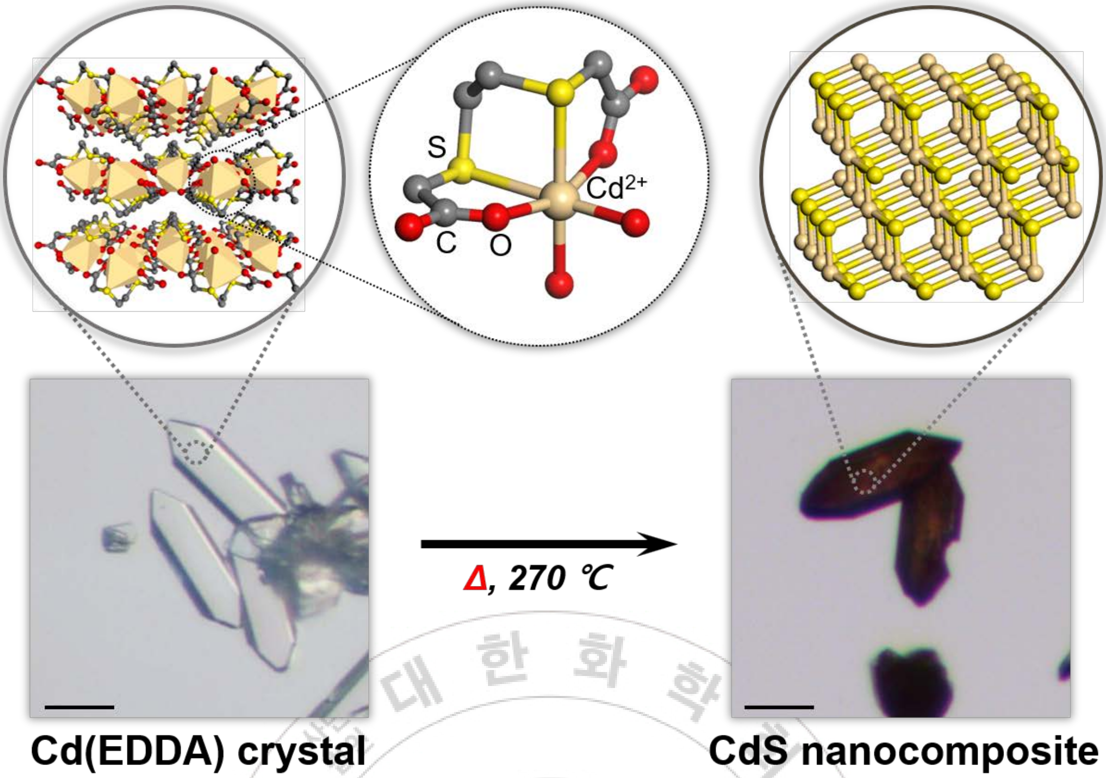
Poster Presentation : **INOR.P-129**
Inorganic Chemistry
Exhibition Hall 1, THU 11:00~12:30

MOF-derived CdS nanocomposite for photocatalytic H_2O_2 production under visible light

Jaehwa Lee, Hoi Ri Moon*

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

In this presentation, we selected CdS as potential photocatalyst under visible light because of its narrow bandgap (2.42 eV) and relatively high conduction band edge position (−0.52 V, vs NHE), and we employed a Cd and S containing metal-organic framework (MOF), [Cd(EDDA)] (EDDA = 2,2’-(ethylenedithio)diacetate), as a precursor for CdS@C nanocomposite. During the thermal conversion, Cd(II) ions were transformed into 5 nm-sized CdS nanoparticles covered with the small amount of carbon (4 wt%). Accordingly, our resultant compound showed efficient H_2O_2 production under visible light just from H_2O and O_2 even in the absence of additional hole scavenger and noble metal co-catalysts. Furthermore, the distinctive feature of this work is the continuous H_2O_2 generation without reaching the saturation point even after 24 h of continuous production. This superior photocatalytic activity to those of earlier reported inorganic photocatalysts might be attributed to the nanosize effect of CdS and thin carbon layers on the surface.


S
C
O
Cd^{2+}
Δ, 270 ℃
Cd(EDDA) crystal
CdS nanocomposite

Poster Presentation : **PHYS.P-130**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Condition in which nanodiscs produced by SMA(styrene:maleic acid)copolymer reliably change the orientation by Ytterbium(Yb^{3+})

Jae-Woong Kim, Dong-Kuk Lee[1,*]

Fine Chemistry, Seoul National University of Science & Technology, Korea
[1]*Department of Fine Chemistry, Seoul National University of Science & Technology, Korea*

In general, bicelle(DMPC/DHPC) is used for structural analysis of membrane proteins using nuclear magnetic resonance(NMR). Because bicelles exist only in certain orientation by the magnetic field. However, surfactants are used to fix membrane proteins of cell membrane in the bicelles. The structure of proteins can be denatured by surfactants. Polymer-based nanodiscs were developed to solve these problems. Polymer-based nanodiscs can directly extract membrane proteins from cell membranes. In this study, we conducted experiments with nanodiscs based on SMA(styrene:maleic acid)copolymer. When structural analysis is performed using solid-state nuclear magnetic resonance(ssNMR), information on at least two orientations is required to interpret the three-dimensional structure. When Ytterbium(Yb^{3+}) is added, the direction of nanodiscs is turned at 90°. Experiments were conducted to find suitable conditions for nanodiscs produced by SMA-based polymers to reliably change the orientation under Yb^{3+} presence. Through ssNMR analysis, information on the orientation of polymer-based nanodiscs was obtained. Nanodiscs produced by SMA-EA are negatively charged, causing them to clump as the concentration of Yb^{3+} increases. $EDTA^{4-}$ was used to address these issues, but not dramatically. Nanodiscs produced by SMA-QA are positively charged, so the orientation was changed reliably by Yb^{3+}.

Poster Presentation : **PHYS.P-131**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Kinetics and Mechanism of 2-Furoyl Chloride

Han joong Koh

General Science Education, Jeonju National University of Education, Korea

Nucleophilic substitution at a carbonyl carbon has been the subject of intensive experimental and theoretical studies. Although the nucleophilic substitution reactions of benzoyl derivatives with anionic as well as nucleophiles have been widely investigated, there is relatively little work reported on the reactions of five-membered hetero-aromatic carbonyl compounds such as thenoyl and furoyl derivatives. We are interested in studying the mechanism of solvolysis of 2-Furoyl Chloride, especially for on going reactions by a dissociation mechanism. In this work, we examined reaction mechanism involved in the solvoysis of 2-Furoyl Chloride, with variety of pure and mixed solvents, eq 1, by determining on the magnitudes of the l and m of the extended Grunwald-Winstein equation, eq 2. 2-Furoyl Chloride + SOH/H_2O —→ (1) log (k/ko) = lNT + mYX + c (2)

Poster Presentation : **PHYS.P-132**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Density Functional Calculation of the warfarin and Vitamin K epoxide reductase

Suhyun Park, **Sangwook Wu**[*]

Department of Physics, Pukyong National University, Korea

Vitamin K epoxide reductase (VKOR), key enzyme for blood coagulation, is the target of the most widely prescribed oral anticoagulant warfarin. Recently, the warfarin binding to the VKOR (TY139A) is revealed by using molecular dynamics simulation based on the three transmembrane model of VKOR. A density functional theory (DFT) calculation verifies a coupled state between the benzene ring of the warfarin moiety and the benzene ring of Tyr139, which supports the three transmembrane model of the VKOR at electronic level. In this presentation, we also discuss possible docking conformations of warfarin inside the binding pocket of VKOR.

Poster Presentation : **PHYS.P-133**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Evaluation of thermal hysteresis activity of ice-binding protein using molecular dynamics simulation

Suhyun Park, Hak Jun Kim[1], Sangwook Wu[*]

Department of Physics, Pukyong National University, Korea

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

Ice-etching experiment and molecular docking demonstrated that two ice-binding proteins (IBP), LeIBP from artic yeast and FfIBP from sea ice bacterium, show different activities in suppressing the growth of ice, leading to different thermal hysteresis (TH) even though they share common features in primary/tertiary structures. In this study, we investigated the ice-binding pattern of the two IBPs to different ice planes, prism and basal plane using all-atom molecular dynamics simulation. Our results provide a fully atomistic description of the difference in TH of two IBPs.

Poster Presentation : **PHYS.P-134**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Branching Ratio of 1-Bromo-3-chlorobenzene Cation

BongGyu Jeong, HyunWook Choi, Jae Kyu Song*, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

The rate constant in chemical reactions provided important information. The reaction rate constant predicts how fast the reaction would take place and could be further applied to the dissociation of the substance of interest. In this reason, measurement of rate constant is highly critical. In our lab, experiments relevant to ternary cluster rate constant have been performed. However, the data of experiments and Phase Space Theory (PST) did not match well. To overcome such problem, we will employ Rice-Ramsperger-Kassel-Marcus (RRKM) theory which is easy to access to interpret the experimental results thoroughly. Experiment of 1-Bromo-3-chlorobenzene Cation (3-BrClBz) will be also carried out to verify if molecules also follow the same tendency. Benzene is one of most useful solvents in chemical reactions. In addition, the halogen group is a well-known functional group. Using Time of Flight (TOF) mass spectroscopy we will investigate the internal energy dependence of branching ratio with Modified RRKM theory. The Branching ratio of 3-BrClBz will be obtained at different internal energies (4.37, 4.55, 4.78 eV). The results of the experiments and Modified RRKM calculations are expected to match well.

Poster Presentation : **PHYS.P-135**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Free Energy Landscape of Coupled Folding and Binding

Song-Ho Chong, Haeri Im, Sihyun Ham*

Department of Chemistry, Sookmyung Women's University, Korea

The most fundamental aspect of the free energy landscape of proteins is that it is globally funneled such that protein folding is energetically biased. Then, what are the distinctive characteristics of the landscape of intrinsically disordered proteins, apparently lacking such energetic bias, that nevertheless fold upon binding? Here, we address this fundamental issue through the explicit characterization of the free energy landscape of the paradigmatic pKID–KIX system. This is done based on unguided, fully atomistic, explicit-water molecular dynamics simulations with an aggregated simulation time of >30 microseconds and on the computation of the free energy that defines the landscape. We find that, while the landscape of pKID before binding is considerably shallower than the one for a protein that autonomously folds, it gets progressively more funneled as the binding of pKID with KIX proceeds. This explains why pKID is disordered in a free state, and the binding of pKID with KIX is a prerequisite for pKID's folding. In addition, we observe that the key event in completing the pKID–KIX coupled folding and binding is the directed self-assembly where pKID is docked upon the KIX surface to maximize the surface electrostatic complementarity, which, in turn, require pKID to adopt the correct folded structure. This key process shows up as the free energy barrier in the pKID landscape separating the intermediate nonspecific complex state and the specific complex state. The present work not only provides a detailed molecular picture of the coupled folding and binding of pKID, but also expands the funneled landscape perspective to intrinsically disordered proteins.

Poster Presentation : **PHYS.P-136**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Extraction of Biomass using Ionic liquid

Insol Jo, Kisub Kim*

Korea National University of Transportation, Korea

As the indiscriminate use of plastics is increasing of interest in micro plastics, materials to replace plastics have come into the spotlight. Researchers become increasingly interested in the development and application of cellulose materials using biomass, so we want to extract cellulose effectively using ionic liquids. In this study, we conduct a study on how to extract cellulose more safely and environmentally friendly. Ionic liquid is non-volatile and is recyclable after use so Ionic liquid recently is in the spotlight. This experiment confirmed that ionic liquid can extract cellulose perfectly and that ionic liquid and cellulose can also be completely separated after extraction. It is expected that by studying the extraction of cellulose using ionic liquids in this study, eco-friendly processes can be newly presented in the relevant field. This was supported by Korea National University of Transportation in 2019

Poster Presentation : **PHYS.P-137**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Observation of the thermal influenced quantum behavior of water solutions near a solid interface

Byoung-Jip Yoon

Department of Chemistry, Gangneung-Wonju National University, Korea

We have observed [1] the anomalous behavior of water near a solid interface by performing capillary flow experiments on water with a silica colloid sample using a high-performance liquid chromatography by accurately varying the temperature, and have analysed the peak shape rigorously. We explained the phenomena as a quantum mechanical behavior of water involved from the characteristic acceptance of thermal displacement according to the Franck-Condon principle. We extended the same experiment in the systems for which urea and salts are dissolved. The newly observed anomalous temperatures were shifted from those of pure water with depending on the dissolved materials and concentrations of the salts. [1] H. Yoon and B. J. Yoon, Sci.Rep. 2018, 8:7016.

Poster Presentation : **PHYS.P-138**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Detection of Azoxystrobin Using Surface-enhanced Raman Scattering

Eungyeong Park, Sila Jin, Yeonju Park, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

Azoxystrobin is a kind of pesticide. It is used to prevent fruits, grain and gardening from insects and fungus. However it can cause water pollution and is harmful human body. Therefore it is important to detect quickly and sensitively. In our research, we tried to detect azoxystrobin based on surface-enhanced Raman scattering (SERS) introduced tyramine signal amplication (TSA). SERS is an ultrasensitive and effective detection method. In TSA based SERS method, a lot of hotspots were generated. Therefore, azoxystrobin could be detected more easily and quickly. Details on the results of detection of azoxystrobin using TSA-based SERS will be discussed in the presentation.

Poster Presentation : **PHYS.P-139**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Spectroscopic studies on thermal behavior of poly(3-hydroxybutyrate-*co*-3-hydroxyhexanoate)

Myeongwon Hwang, Yeonju Park, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

Poly(3-hydroxybutyrate-*co*-3-hydroxyhexanoate) (PHBHx), a biodegradable polymer, is widely studied as a potential substitute for petroleum-based thermoplastics. To investigate melting and crystallization processes of PHBHx with different 3-Hx molar fraction, we used infrared reflection absorption spectroscopy (IRRAS) and two-dimensional correlation spectroscopy (2D-COS). Details on the results of thermal behavior of PHBHx using IRRAS and 2D-COS will be discussed in this presentation.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Poster Presentation : **PHYS.P-140**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Study of Reusable Photocatalyst for Organic Dye Molecule Degradation

Sila Jin, Lei Chen[1], Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea
[1]*College of Chemistry, Jilin Normal University, China*

Organic dyes are widely used in industry, but because they cause water pollution, they must be degraded with little or no toxicity. However, it is very stable in water and requires degradation with a catalyst. Photocatalyst that is active in the visible region has the advantage of utilizing solar-light. Therefore, research on the development of visible-light responsive photocatalyst is being actively conducted. The strong magnetization of Fe_3O_4 is economical because it can be easily separated and reused. In this study, we fabricated a stable and improved photocatalyst by adding TiO_2 and Au nanoparticles to Fe_3O_4 nanoparticles. The prepared photocatalyst was characterized by TEM, EDX, XRD, and XPS, and the degradation of organic dyes was observed using UV-Vis and Raman spectroscopy. Details on its characterization and analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-141**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Methodology development of ligand screening by using NMR spectroscopy

Yoonjin Um, Young Kee Chae*

Department of Chemistry, Sejong University, Korea

We have been developing a new screening approach by employing a supramolecular complex and NMR-based metabolomics. Our approach depends on a very fast exchange between free and bound state of the ligand. And it is based on the hypothesis that any molecule that binds to a very large target protein will lose its NMR signal due to a very slow tumbling rate, which is, in fact, a fundamental phenomenon of NMR spectroscopy. We also borrowed the concept of metabolomics which dealt with a mixture of many compounds. That is, instead of trying different compounds to the target protein one by one, we use a mixture of many compounds and look for a binder once and for all. Our approach to making a very large target protein is through the formation of a supramolecular complex by using a polypeptide (ELP) that tends to aggregate, not get denatured, at slightly elevated temperatures. We selected the maltose binding protein (MBP) to prove our hypothesis. We predicted that MBP-ELP can detect analogues of maltose by this screening system. And we will also apply this method to compound complexes. We hope this new method will facilitate the finding of lead compounds without relying on a large chemical library. This work has been supported by Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2017R1D1A1A02017545).

Poster Presentation : **PHYS.P-142**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Analyzing Turkish Propolis from a variety of Geographical Origins by Using NMR Spectroscopy

Hakbeom Kim, Young Kee Chae[1,*]

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

The main effects of propolis (or bee glue) products are known to be antibacterial, antioxidant and anti-cancer. Propolis is a mixture of honey bee saliva, beewax, and exudate from various plant sources. We want to determine which constituents of propolis are responsible for such beneficial effects by analyzing extracts from propolis raw materials. We are also trying to find a correlation between the effects and geographical nature of Turkish propolis. As a first step, we started with commercially available propolis products in two forms, liquid and powder. And next, we extracted propolis raw materials in three methods, boiling water, 70% ethanol, 100% ethanol. We also analyzed the extracts of propolis by NMR spectroscopy. We hope that this work will help the bio-industry by providing information regarding the effects and origins. This work was supported under the framework of international cooperation program managed by National Research Foundation of Korea (NRF-2018K2A9A1A06065371).

Poster Presentation : **PHYS.P-143**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

DFT study of dissociative electron attachment to several aryl halides

Jangho Park, Namdoo Kim*

Division of Chemistry, Kongju National University, Korea

Aryl halides like 1,3-dichloro-2-bromobenzene(DCBB), 1,3-dibromo-2-iodobenzene(DBIB), 1,3-dichloro-2-iodobenzene(DCIB) were investigated theoretically using DFT calculation. Iodine was dissociated from the parent molecule in DCIB and DBIB upon electron binding, while Br atom in DCBB anion was not dissociated in B3LYP and B3P86 methods. However, in case of O3LYP, less electronegative halogen atoms (Br and I in the DCBB and DCIB, DBIB, respectively) were dissociated from the parent molecule upon electron binding. Mulliken charge analysis revealed that an approaching electron was mostly localized to the less electronegative halogen atom. In addition, MO analysis showed that an extra electron occupies anti-bonding orbital between these less electronegative atoms and carbon which results in elongation of the bond length. Vertical detachment energies (VDE) of all three anions seem to be much higher than adiabatic electron affinities (AEA) which tell us dramatic geometry change during anion formation.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Theoretical study of halogen-substituted benzene molecules upon electron attachment

Minwoo Jang, Namdoo Kim*

Division of Chemistry, Kongju National University, Korea

We investigated three halogen-substituted benzene molecules and anions (1,3-dibromo-2-chlorobenzene (DBCB), 1,3-diiodo-2-chlorobenzene (DICB) and 1,3-diiodo-2-bromobenzene (DIBB)) using DFT calculations. B3LYP, B3P86 and O3LYP gave us the same results that almost half of an extra electron localized to the less electronegative halogen atoms. Molecular orbital analysis revealed that a negative charge occupies anti-bonding orbitals between these halogen atoms and carbon atom resulting decrease of the bond order and elongation of the bond length. Difference between vertical detachment energies (VDE) and adiabatic electron affinities (AEA) is nearly 1.0 eV, 0.9 eV and 0.8 eV for DBCB, DICB and DIBB, respectively.

Poster Presentation : **PHYS.P-145**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Development of MATLAB Code for Calculating Reorganization Energy of Benzene and Anthracene Molecules from Their Optimized Geometries in Cartesian Coordinates

Hyeok Yun, Young-Hwa Choi, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

We have developed a MATLAB code to calculate electron/hole hopping reorganization energies of molecules from their force constant matrices and optimized geometries in Cartesian coordinates in Gaussian output files. The reorganization energy can be calculated as the sum of vibrational potential energies, in harmonic oscillator approximation, corresponding to displacements along normal mode vectors. In order to extract vibrational modes and angular frequencies of a molecule, we first solved eigenvalue problem of its mass-weighted force constant matrix. We then translated atoms' position for its center of mass to be the origin and aligned its molecule-body axes to its principal axes. Under the assumption that its principal axes are kept fixed before and after charge transfer, we calculated the displacements of neutral and charged states along their normal mode vectors. Optimized geometries and force constant matrices of neutral and charged states were calculated with Gaussian 03W and Gaussian 16W packages, where DFT-B3LYP method and 6-31G(d,p) basis were used.

References:
1. A. Klimkans, S. Larsson, *Chemical Physics* **1994**, *189*, 25
2. Y. H. Park, Y. H. Kim, S. K. Kwon, I. S. Koo, K. Yang, *Bull. Korean Chem. Soc.* **2010**, *31*, 1649

Benzene		**Reorganization energy (eV)**					
		Electron hopping			Hole hopping		
Gaussian ver.	Basis	λ_N	λ_C	λ_{total}	λ_N	λ_C	λ_{total}
G 92 $^{1)}$	6-31G	0.2712	0.2807	0.5519	-	-	-
G 03	6-31G(d,p)	0.2206	0.2292	0.4497	0.1617	0.1859	0.3475
G 16	6-31G(d,p)	0.2175	0.2410	0.4585	0.1587	0.1712	0.3299

Anthracene		**Reorganization energy (eV)**					
		Electron hopping			Hole hopping		
Gaussian ver.	Basis	λ_N	λ_C	λ_{total}	λ_N	λ_C	λ_{total}
G 98 $^{2)}$	6-31G(d,p)	0.099	0.101	0.200	0.068	0.069	0.137
G 03	6-31G(d,p)	0.0985	0.1013	0.1998	0.0667	0.0675	0.1342
G 16	6-31G(d,p)	0.0957	0.1002	0.1959	0.0664	0.0683	0.1347

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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **PHYS.P-146**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Growth of Carbon Nanotube by Microwave Plasma Enhanced Chemical Vapor Deposition(MPECVD) using Nickel Catalyst

Yu Jin Song, Changsoon Huh*

Applied Chemistry, Dong-Eui University, Korea

We have grown carbon nanotubes (CNTs) with a microwave plasma enhanced chemical vapor deposition (MPECVD) method, which has been regarded as one of the most promising candidates for the synthesis of CNTs. We have used argon (Ar) and hydrogen (H2) gas and acetylene (C2H2) as precursor for the growth of CNTs. Ni catalytic layer (10 nm thick) were deposited on the Ti coated Si substrate by RF magnetron sputtering method. In this work, we report the effects of heat treatment on the growth of CNTs, in which we have pretreated the Ni catalytic layer in different temperature (600, 650, and 700 ℃) and moderate microwave power (400W). We investigated the effect of pretreatment temperate of the Ni catalyst layer on the growing characteristics of MWCNTs. Adhesion of Ni (10 nm) is shown to influence the growth characteristics with Ni used as active catalysts. The images show Ni catalytic layer diameter and density are varied dependent on their pretreatment conditions. In order to determine the properties of CNTs, we performer scanning electron microscope(SEM), transmission electron microscopy(TEM), atomic force microscopy(AFM), and X-ray photoelectron spectroscopy(XPS) analysis.

Poster Presentation : **PHYS.P-147**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Stochastic Kinetics of Nanocatalytic Systems

Jingyu Kang, Jaeyoung Sung[1,*]

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

Catalytic reaction events occurring on the surface of nanoparticle constitute a complicated stochastic process. Although advances in modern single molecule experiments enable direct measurements of individual catalytic turnover events occurring on a segment of single nanoparticle, it is yet to be known how the catalytic turnover time distribution is related to microscopic dynamics of catalytic reactions. Here, we present a general theory of the turnover time distribution for a nanoparticle catalyst and apply it to exactly solvable models of nanocatalytic systems. From our model study, we find that communication among catalytic sites greatly increases the randomness in the catalytic turnover time and dramatically affects the sign and reactant concentration dependence of the randomness parameter of nanoparticle catalytic reactions. Ubiquitous heterogeneity of nanoparticle size is an additional source of randomness in the catalytic turnover time. This work enables a quantitative analysis of the catalytic turnover time distribution for nanocatalytic systems and other catalytic systems with multiple catalytic sites.

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Poster Presentation : **PHYS.P-148**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Poly(acrylic acid)-rhodamine coated gadolinium oxides nanoparticles as dual functional MRI – cell labeling agents

Son-Long Ho, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this work, gadolinium oxides nanoparticles which were coated by poly(acrylic acid)-rhodamine showed high T1 and T2 relaxivities and low cytotoxicity to cells. Gd NPs were well coated and have small hydrodynamic size, which help Gd NPs to be fully excreted from the body through the renal system to avoid any danger such as nephrogenic systemic fibrosis. Due to the presence of rhodamine moiety, Gd NPs also showed fluorescent and pH-responsive property which can be used to differentiate normal and cancer cells in vitro.

Poster Presentation : **PHYS.P-149**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Amorphous carbon-coated ultrasmall Gd_2O_3 nanoparticles used for dual-modal imaging agent

Huan Yue, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this study, the amorphous carbon-coated ultrasmall gadolinium oxide ($C@Gd_2O_3$) core-shell nanoparticles (shell: amorphous carbon; core:Gd_2O_3) were synthesized through a facile two-step process in aqueous solution. Because carbon is biocompatible, non-toxic, and photoluminescent in the visible region. The ultra-small $C@Gd_2O_3$ NPs with a narrow size distribution in the range of d_{avg} = 3.1 nm and a_{avg} = 18.9 nm that had an excellent colloidal stability, very high r1 value (16.26 $s^{-1}mM^{-1}$; r2/r1 = 1.48), and exhibited photoluminescence in the visible region. In vitro non-toxic confirmed by both DU145 and NCTC1469 cell lines. Additionally, a high contrast in vivo positive magnetic resonance images and micrometer-scale fluorescence images were obtained, demonstrating that the potential of the ultrasmall $C@Gd_2O_3$ NPs could be used as a dual-mode MR and florescence imaging agent.

Poster Presentation : **PHYS.P-150**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Size-controlled one-pot polyol synthesis and characterization of D-glucuronic acid-coated ultrasmall BiOI nanoparticles as potential x-ray contrast agent

Adibehalsadat Ghazanfari, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Iran

A polyol method is extremely useful for preparimg metal-containing nanoparticles coated with hydrophilic and biocompatible ligands for biomedical applications. In this study, D-glucuronic acid coated BiOI nanoparticles were prepared in one-pot using this method. The particle diameter was controlled by varying the solvent volume such that the particle diameter decreased with increasing solvent volume: nanoparticles with average diameters of 1.9 (ultrasmall) and 6.1 nm were prepared at two solvent volumes. The x-ray attenuation properties of the ultrasmall nanoparticles were investigated because of their suitability for in vivo biomedical applications. D-glucuronic acid-coated ultrasmall BiOI nanoparticles were superior to the commercial molecular iodine contrast agent Ultravist® in terms of x-ray attenuation, and showed the highest x-ray attenuation efficiency (η) of ～21 HU/mM [Bi] that has ever been reported thus far, proving their potential as an extremely powerful x-ray contrast agent.

Poster Presentation : **PHYS.P-151**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Cyclic RGD conjugated ultrasmall gadolinium oxide nanoparticles as tumor T1 targeting MRI contrast agents

Mohammad Yaseen Ahmad, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this study we investigate tumor targeting T_1 magnetic resonance imaging (MRI) contrast agents. The ultrasmall Gadolinium Oxide 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 (r1= 10.0 - 18.7 s^{-1} mM^{-1} and r_2/r_1 = 1.4 - 1.7) higher than those of commercial Gd-chelates.

Poster Presentation : **PHYS.P-152**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Study of D-glucuronic acid-coated Ultrasmall Paramagnetic Ln_2O_3 (Ln = Tb, Dy, and Ho) Nanoparticles: Water Proton Relaxivities at High Field Magnetic Resonance Imaging

Shuwen Liu, Gang Ho Lee[1,*]

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

Contrast agents have been used since beginning in Magnetic resonance imaging (MRI) to improve the image contrast, through their influence in water proton relaxation times. The paramagnetic lanthanide elements served as valuable contrast medium as they possess excellent magnetic properties useful for MRI while some of these elements have additional optical properties and can serve as fluorescence imaging (FI) agents as well. Herein, we synthesized D-glucuronic acid-coated ultrasmall Ln_2O_3 (Ln = Tb, Dy, and Ho) nanoparticles by a polyol method to investigate their water proton relaxivities at higher magnetic field (9.4 T). Despite their ultrasmall diameters (~2 nm), all the nanoparticles showed unsaturated but appreciable magnetization of ~4 emu/g at an applied field of 1.8 T at room temperature, and consequently, high transverse water proton relaxivities (r_2) with negligible longitudinal water proton relaxivities (r_1), thus being eligible for use as T_2 contrast agents in MRI. In addition, D-glucuronic acid-coated ultrasmall Tb_2O_3 nanoparticles exhibited fluorescence in the green region, indicating that they may serve as a dual imaging agent in FI and T_2 MRI.

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Poster Presentation : **PHYS.P-153**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

DFT study of covalent bond formation upon electron attachment to CO_2 -carboxy pyridine

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Carbon dioxide is an extremely inert molecule in neutral state at room temperature. Previous study demonstrated that carbon dioxide could form covalent bond with N-heterocyclic compounds like pyridine, pyrimidine, pyrazine and triazine when they became an anion at low temperature. Here, we studied interaction between carbon dioxide and pyridine which has a carboxyl group at o-, m- and p- position, respectively using DFT methods. Carbon dioxide formed covalent bond with N atom in case of m- and p-carboxy pyridine while o- isomer did not. It seems that repulsion between O atoms in carbon dioxide and –COOH played a key role for this result due to short distance. m- and p-pyridine- CO_2 complexes showed large vertical detachment energy (VDE) shift upon electron attachment. In addition, linear CO_2 became bent which is consistent with previous studies.

Poster Presentation : **PHYS.P-154**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structure characterization of $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ thin films (x=0.02, 0.05) incorporated with different additives using x-ray reflection and diffraction

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Neutron Science Division, Korea Atomic Energy Research Institute, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*
[2]*Solar Energy Materials, Korea Research Institute of Chemical Technology, Korea*

We have investigated the effect of different additives on thin film structure and morphology of ((formamidinium (FA) or $HC(NH_2)_2)PbI_3)_{1-x}$((methylammonium (MA) or $CH_3NH_3PbI_3)PbBr_3)_x$ (x=0.02 or 0.05) thin films using specular x-ray reflection (XRR) and low-angle x-ray diffraction(XRD). 50 nanometer-thick $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ thin films were synthesized by spin-coating on Si substrate with a surface dimension of 1×1 $inch^2$ and three different kinds of additives such as MACl and 5 mol% CsI and 5 mol% RbI were considered. Further details on sample synthesis can be found in reference [1]. Kiessig interference fringe owing to total film thickness in XRR data is clearly observed in MACl-added $(FAPbI_3)_{1-x}(MAPbBr_3)_x$films only, indicating that they are pin-hole free, continuous, and interface/surface roughness is not so rugged over Si substrate. Besides, there exists a very thin layer with a few nanometer thickness between substrate and $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ sublayers for all the samples irrespective of additives. XRR data analysis reveals that this thin layer is likely to be PbI_2. Low angle XRD shows that a very strong α-$FAPbI_3$ (100) peak at 2θ=13.9º is observed but δ-$FAPbI_3$ (100) peak at 2θ=11.7(8)º is not in MACl-added $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ films. Meanwhile, both α-$FAPbI_3$ and δ-$FAPbI_3$ are observed and α-$FAPbI_3$ (100) peak intensity is significantly reduced in CsI or both CsI and RbI-added $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ films due to the relatively worse surface morphology. It should be noted that PbI_2 (001) phase at 2θ=12.7 º is present for all the samples. Time-dependent XRD data show that α-$FAPbI_3$ peak remains intact even though they has been unencapsulated and exposed to a humid air of relative humidity of around 50%. However, XRR unambiguously exhibits that the interdiffusion between $(FAPbI_3)_{1-x}(MAPbBr_3)_x$ and PbI_2(001) sublayers takes place over a period of about one month. We suggest that a combination of XRR and XRD can be effective experimental tools to characterize the structure of the inorganic-organic perovskite thin

films.Reference[1] N. J. Jeon, J. H. Noh, W. S. Yang, Y. C. Kim, S. Ryu, J. Seo & S. I. Seok, Compositional engineering of perovskite materials for high-performance solar cells, Nature 517 (2015) 476-480

Poster Presentation : **PHYS.P-155**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Simulations on polymer loop formation kinetics in heterogeneous porous media

Seulki Kwon, Bong June Sung*

Department of Chemistry, Sogang University, Korea

A variety of macromolecules such as proteins and cytoskeleton structures occupy up to 40% of the cytoplasmic volume of cells. Such diverse macromolecules make the cell cytoplasm not only structurally heterogeneous but also dynamically heterogeneous: some macromolecules may diffuse freely inside cell cytoplasm at a certain time scales but others hardly diffuse. While the effects of the crowdedness and structural heterogeneity on the reaction kinetics have been investigated extensively, studies on the effects of the heterogeneous dynamics are limited. In this study, we employ a simple model of mixtures of mobile and immobile matrix particles, and tune the degree of dynamic heterogeneity by changing the fraction of immobile matrix particles. We investigate the loop formation of a single polymer chain as a model reaction by performing Langevin dynamics simulations. As the volume fraction of immobile matrix particles reaches a critical value at the percolation transition, the reaction kinetics becomes significantly heterogeneous and the survival probability distribution of the chain loop formation becomes stretched-exponential. We also find that heteroge- neous reaction rate near the percolation transition is closely related to the structures of local pores in which the polymer is confined.

Poster Presentation : **PHYS.P-156**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

The effect of silicon quantum dot on density of states of conjugated capping groups

Ji Young Bang, Young-Hwa Choi[1], Hyun-Dam Jeong[1,*]

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

As for electrons in molecule or quantum dot with silicon-carbon interface, we can adopt the viewpoint of two sets of eigenvectors, instead of treating delocalized states over entire molecule or quantum dot, where density of states (DOS) of one part is affected by that of the other part. We first divided entire molecule into ‘stimulator’ which is influencing and ‘responsor’ which is affected. Then we imposed Gaussian functions with a natural broadening on eigenstates of the stimulator to make its Green’s function. We combined it with coupling matrix to provide self energy matrix (molecular stimulation function), which was used to obtain Green’s function of the responsor (molecular responsor function) generating its DOS. Ambiguity of initial guess at standard deviation value of the Gaussian function was overcome by adjusting electron number of the responser to one obtained from its density matrix. Optimized geometries of molecules or silicon quantum dots and their overlap, Fock and density matrices were calculated with Gaussian 16 package, where DFT□ B3LYP method and 6-31G(d,p) basis were used. We have developed a Matlab code to calculate the Green’s functions, self energy matrices, and DOS, whose applicability were first confirmed on the investigation of the effect of silicon quantum dot on DOS of conjugated capping groups.

Poster Presentation : **PHYS.P-157**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Electronic Coupling in π-Conjugated Molecule-Bridged Silicon Quantum Dot Clusters Synthesized by Sonogashira Cross-Coupling Reaction

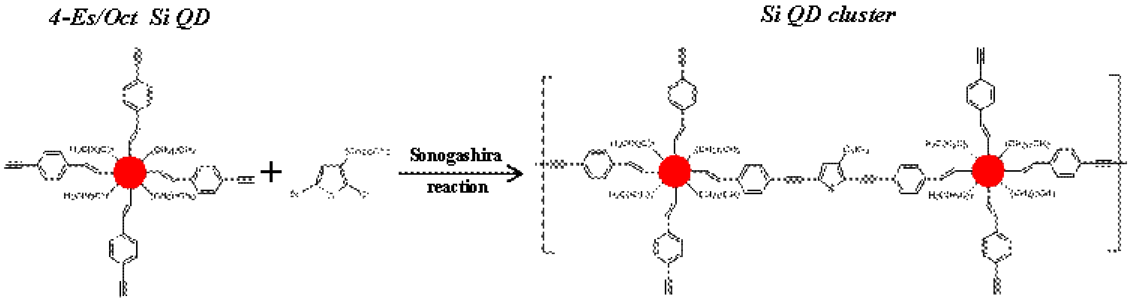
Young-Hwa Choi, Hyun-Dam Jeong*

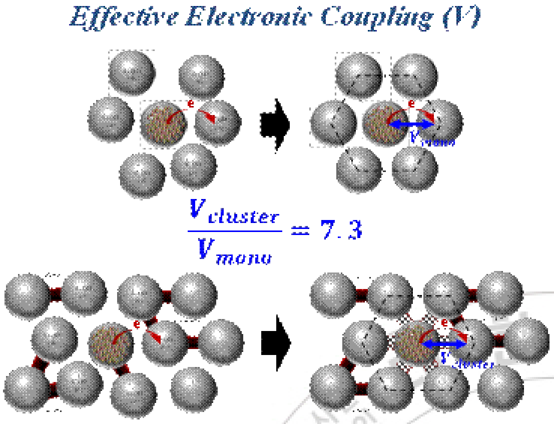
Department of Chemistry, Chonnam National University, Korea

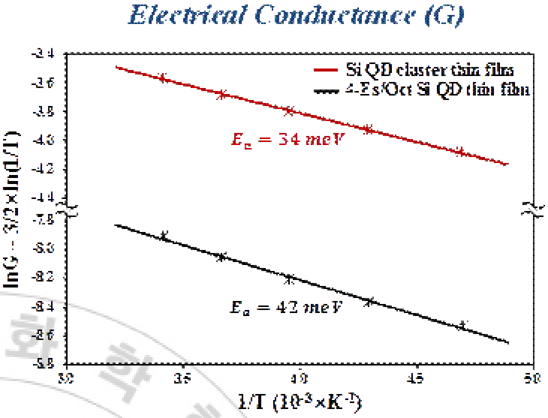
π-Conjugated molecule-bridged silicon quantum dot (Si QD) clusters were first synthesized by Sonogashira cross-coupling reaction between 4-ethynylstyryl and octyl co-capped Si QDs (4-Es/ Oct Si QDs) and 2,5-dibromo-3-hexylthiophene. The formation of Si QD clusters was confirmed by field emission transmission electron microscopy. The electronic coupling between the QDs in the Si QD cluster is significantly enhanced as compared with that for 4-Es/Oct Si QDs, which is verified from the red shift in ultraviolet−visible absorption and photoluminescence spectra of the Si QD cluster with the possibility of exciton transport, the increased charging effect found in the core-level photoemission spectra, the shift to lower binding energy of the valence band photoemission spectrum, and more decisively, the increase in electrical conductance of the Si QD cluster thin film. To investigate the physical origin of the temperature dependence of the electrical conductance, we have merged the microscopic viewpoint, Marcus theory, on the electron transfer (W) between the adjacent QDs, with macroscopic concepts, such as the conductance (G), mobility (μ), and diffusion coefficient (D). The effective reorganizational energies of charge transfer between the neighboring Si QDs in 4-Es/Oct Si QD and Si QD cluster thin films are estimated to be 170 and 140 meV, respectively, while the ratio of the effective electronic coupling of the latter to that of the former is determined to be 7.3:1.

Reference:

1. T. -H. Le, Y. -H. Choi, K. -J. Kim, H. -D. Jeong, *ACS omega* **2019**, *4*, 3133-3145


4-Es/Oct Si QD
Si QD cluster
+
Sonogashira reaction


Effective Electronic Coupling (V)
e
V_{mono}
$\frac{V_{cluster}}{V_{mono}} = 7.3$
e
$V_{cluster}$


Electrical Conductance (G)
Si QD cluster thin film
4-Es/Oct Si QD thin film
$E_a = 34\ meV$
$E_a = 42\ meV$
lnG – 3/2×ln(1/T)
-3.4
-3.6
-3.8
-4.0
-4.2
-4.4
-7.8
-8.0
-8.2
-8.4
-8.6
-8.8
3.0
3.5
4.0
4.5
5.0
1/T (10^{-3}×K^{-1})

Poster Presentation : **PHYS.P-158**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Quantum Chemical Calculation of Electronic Coupling for Studying Non-adiabatic Electron Transfer in Silicon Quantum Dot Dimer

Young-Hwa Choi, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

We established theoretical formalism and computational method to describe non-adiabatic bridged-mediated electron transfer in silicon quantum dot (Si QD) dimer system. In the Si QD dimers with various organic/inorganic bridging groups, such as poly(p-phenylene vinylene), poly(p-phenylene ethynylene) and polysiloxane, electronic couplings between QDs were estimated from Fock matrix of the QD dimer and eigenstates of donor/acceptor QDs. The Fock matrices were obtained by quantum chemical calculation using DFT method at B3LYP/6-31G(d,p) or LanL2DZ levels in Gaussian 16 package and the electronic coupling values were calculated with Matlab code based on Green's function.

Poster Presentation : **PHYS.P-159**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Predicting protein-ligand binding affinity using the ensemble of 3D-convolutional neural networks

Yongbeom Kwon, Juyong Lee*

Department of Chemistry, Kangwon National University, Korea

Accurate prediction of the binding affinity of a protein-ligand complex is essential for efficient and successful rational drug design. In this work, a new neural network model that predicts the binding affinity of a protein-ligand complex structure is developed. Our new model predicts the binding affinity of a complex using the ensemble of multiple independently trained networks that consist of multiple channels of 3D convolutional neural network[1] layers. Our model was trained using the 3740 protein-ligand complexes from the refined set of the PDBbind[2] database and tested using the 270 complexes from the core set. The benchmark results show that the correlation coefficient between the predicted binding affinities by our model and the experimental data is higher than 0.72, which is comparable with the state-of-the-art binding affinity prediction methods.[3] In addition, our method also ranks the relative binding affinities of possible multiple binders of a protein quite accurately. Last, we measured which structural information is critical for predicting binding affinity.

References

[1] LeCun, Y. et al., Nature, 521 (2015), 436–444.

[2] Liu, Z. et al., Acc. Chem. Res., 50 (2017), 302–309.

[3] Su, M. et al., J. Chem. Inf. Model., 59 (2019), 895–913.

Poster Presentation : **PHYS.P-160**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Associative Electron Attachment in Dianionic N-doped Graphene Moiety-CO2 Complexes

ChangJun Park, **Sang Hak Lee***

Department of Chemistry, Pusan National University, Korea

Nitrogen-containing polycyclic aromatic hydrocarbon (PAH) is the single basic moiety in N-doped graphene, the only metal-free catalyst reported to date to successfully produce the oxygen reduction reaction. N-doped graphene is quite promising as a material to increase the efficiency of oxygen reduction. In addition, it is known that when carbon dioxide is added to azabenzene, there will be an associative chemical reaction upon electron attachment between the anionic nitrogen atoms in the azabenzene and the carbon atom in the carbon dioxide; however, it has previously been reported that when there are more nitrogen atoms in the small aza-benzene moiety, the associative reaction does not always occur. In this study, we carried out a theoretical simulation to determine whether more electrons increase the CO2 reductive reactivity of nitrogen-containing polycyclic aromatic hydrocarbon. We found that even though an associative chemical reaction between nitrogen atoms in N-PAH and carbon atoms in carbon dioxide did not occur in anionic complexes of N-PAH and carbon dioxide, chemical reactions did occur in all nitrogen atoms of these complexes when we added an extra-excess electron. Therefore, we conclude that the efficiency of CO2 reduction will be increased in nitrogen atoms when more electrons are added to increase their anionic properties.

Poster Presentation : **PHYS.P-161**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Photocatalytic decomposition of Acetaldehyde and NOx over TiO_2 catalysts under visible light

Shufang Zhao, Soong Yeon Kim, Byeong Jun Cha, Saqlain Shahid, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

As-received TiO_2 (commercial P25), 750 ºC annealed TiO_2, and 750 ºC annealed Fe deposited TiO_2 (FeO_x/TiO_2, prepared by temperature regulated chemical vapor deposition) photocatalysts were used for photocatalytic decomposition of acetaldehyde and NOx under visible light. As-received TiO_2 almost did not show photocatalytic activity for acetaldehyde decomposition under visible light, however, 750 ºC annealed TiO_2 showed increased photocatalytic activity for acetaldehyde decomposition and when a very small amount of Fe loaded on TiO_2, the activity became maximized. In addition, NOx removal result of all photocatalysts showed different photocatalytic activity under visible light, which followed as ISO 221971-1. Comparing the three kinds of samples, FeO_x/TiO_2 can absorb more visible light so it showed high activity which may be attributed to synergistic effect and minimum electron hole recombination caused by the Fe ions incorporated into the crystal lattice of TiO2. We suggested FeO_x loaded on the TiO_2 improved its photocatalytic performance for the photodegradation of gaseous VOCs and removal of NOx.

Poster Presentation : **PHYS.P-162**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Two state diffusion of PCNA in DNA skybridge

Gyunam Park, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

We investigated that proliferating cell nuclear antigen(PCNA) which plays several role on DNA replication and translesion freely diffuse on DNA skybridge attached on both side of top of nano-fabricated twin tower. We observe that MSD(Mean-squared displacement) of PCNA diffusion trajectory shows saturation to point which not predicted by experimental DNA length. And PCNA is known as diffusing on two state that the one is sliding mode, the other is hopping mode. Therefore, we set a model for PCNA diffusion by two state diffusion on 1D finite box. By theoretical approach, we can explain diffusion dynamics of PCNA by fitting MSD and NGP(Non-Gaussian parameter). So, we confilm that PCNA diffuse on two diffusion state. And there is a protein named PAF15 which known as decreasing diffusivity of PCNA. We compare dynamics of PCNA and PCNA-PAF15 complex. We shows that PAF15 not only decreases static diffusivity of PCNA but also decreases dynamic change in two state dynamics.

Poster Presentation : **PHYS.P-163**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Reaction pathway of the surface reaction of cis-2-butene-1,4-diol on semiconductor surfaces

Eunkyung Hwang, Jeonghui Choi[1], Do hwan Kim[1,*]

Dasan University College, Ajou University, Korea
[1]*Department of Chemistry Education, Chonbuk National University, Korea*

The reaction pathway for the adsorption of cis-2-butene-1,4-diol on Ge(100) surface was investigated using density functional theory calculations. The dissociation of the two hydroxyl group in cis-2-butene-1,4-diol may be either O-H or C-O dissociation. Possible pathways from the molecular adsorption to the dual dissociative configurations were considered and the activation barriers in the pathways were also calculated. Our results suggest that dual dissociative products may be formed with small barrier and the bridged configurations may be confined to a dimer row or may be located over two dimer rows.

Poster Presentation : **PHYS.P-164**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Study on Luminescence Mechanism of Upconversion Materials Using Pulse Modulation

Lim SooYeong, Chan Ryang Park[1], Hyung Min Kim*

Department of Bionano Chemistry, Kookmin University, Korea
[1]*Department of Chemistry, Kookmin University, Korea*

Upconversion materials have features which convert low energy light into high energy light have been applied in such as solar cells and bioimages. Among them, $NaYF_4$: Yb^{3+}, Er^{3+} phosphors attracted great attention due to the highly efficient upconversion process. Upconversion spectrum was influenced by the composition of the phosphor, power density of the laser, and excitation time. However, systematic study of the upconversion mechanism has not been reported. In this study, a pulse modulation system (PMS) was introduced for the photophysical analysis of energy accumulation and relaxation. In the modulation experiments of pulse width and interval, it can be seen that it takes 5ms for the hot phosphor to cool down completely. And the intermediate state of $^4I_{13/2}$ proves to be filled with high temperature phosphors and affect the upconversion emission color. These results provide clues to the reason for discussion of the various red upconversion mechanisms of $NaYF_4$: Yb^{3+}, Er^{3+}.

Poster Presentation : **PHYS.P-165**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Adsorption characteristic of a CNT sponge preconcentrator for gaseous samples

Yeonhee Jang, Yeong Sik Seon, Kwang woo Jung*

Department of Chemistry, Wonkwang University, Korea

A carbon nanotubed sponge (CNTS) based GC preconcentrator that accumulates trace amounts of VOCs in air sample has been developed. CNTS was fabricated using the spray pyrolysis chemical vapor deposition (CVD). CNTS has distinct adsorption capacity for each adsorbates by interactions with the CNTS depending on various physical-chemical properties. (molecular structure, vapor pressure, polarity, etc.) The roll-up phenomenon was observed in the breakthrough curve of mixture compounds, which fits well into the multicomponent system of Yoon’s equation. Furthermore CNTS has low affinity against humidity and low interference from other gases such as NO_x and NH_3. Therefore CNTS preconcentrator is especially suitable for a portable GC that uses an ambient air as a carrier gas.

Poster Presentation : **PHYS.P-166**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

The adsorption behavior of guanine on Ge(100) surface : A theoretical study

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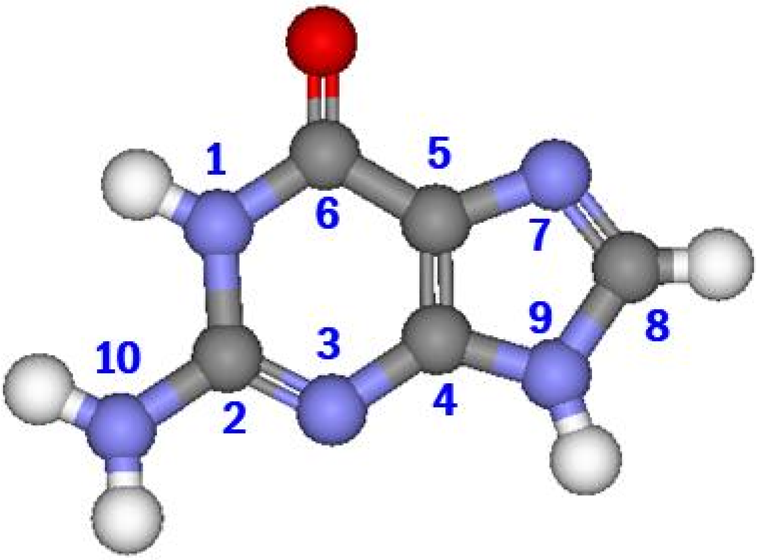
The adsorption structure and reaction mechanism of Guanine on Ge(100) surface was investigated using density functional theory (DFT) calcualation.We found that the most stable adsorption configuration of guanine on Ge(100) surface is “N(1)-H dissociation through an O dative bonded structure”. In the reaction pathway from O-dative bonded structure to N(1)-H dissociation configuration, the energy of its transition state is slightly higher than that of reactant.It means that theadsorption structure of guanine on Ge(100) surface is "N(1)-H dissociation through an O dative bonded structure" because the reactant can easily overcome its relative low activation barrier.



Poster Presentation : **PHYS.P-167**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Photoemission spectroscopy study of H_2O adsorbed on ZIRLO^{TM} cladding

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Adsorption behavior of H_2O on ZIRLO^{TM} cladding was investigated using a photoemission spectroscopy (PES) at pohang accelerator laboratory (PAL). Analysis of Zr 3*d*, O 1*s*, C 1*s*, and Sn 3*d* PES spectra obtained from intact ZIRLO^{TM} showed the surface compositions of O^{2-}, OH^-, H_2O, metal carbide, C, Sn, and SnO_2 features. After the deposition of H_2O on ZIRLO^{TM}, the relative population of Zr composition decreased while total Zr oxides increased. Furthermore, after heating of the sample at 300°C, we observed that the decomposition of some Zr oxides occurred.

Poster Presentation : **PHYS.P-168**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

A microscopic view on nonlinear mechanical responses of glassy polymer nanofibers

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Polymer fibers are promising materials for various applications due to their unique thermal and mechanical properties. Recent experiments showed the mechanical properties of polymer glassy nanofibers differ from those of bulk polymer glasses. For example, Young's modulus of Nylon-11 nanofibers increases with decreasing fiber diameter. The complex mechanical behaviors of glassy polymer fibers, however, are yet to be understood at the molecular level. In this work, we conduct molecular dynamics simulations to investigate nonlinear mechanical behaviors of glassy polymer nanofibers. We apply uniaxial deformation on glassy polymer fibers under constant strain rate. We show that, in our simulations, glassy polymer nanofibers exhibit nonlinear mechanical responses: elastic regime, stress overshoot regime, plastic flow regime, and strain hardening regime. We find that large deformation enhances non-affine behaviors of glassy materials, which causes nonlinear mechanical responses of polymer fibers after the yield point. Finally, we show that the magnitude of the non-affine displacement in surface is larger than the magnitude of the non-affine displacement in other regions.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Density functional theory study on adsorption behavior of L-vailne on Ge(100) suface

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The adsorption behavior of L-valine on the Ge(100) surface was investigated by density functional theory (DFT) calculation. Because L-valine contains a carboxyl (-COOH) group and an amino (-NH_2) group, two oxygen and one nitrogen atoms in these functional groups react with Ge(100) surface. Therefore, we calculated three possible reaction pathways participating in these oxygen and nitrogen atoms to study which pathway is more favorable among them; The first is the O-H dissociation (C=O) pathway via the carbonyl oxygen dative-bonded state, the second is O-H dissociation pathway via hydroxyl oxygen dative-bonded state, and the last third is the N-H dissociation pathway via the nitrogen dative-bonded state. As a result of the DFT calculations, we found that “intrarow O-H dissociated and N dative-bonded structure” is the most stable structure of L-valine on Ge(100) surface, which occurred through O-H dissociation (C=O) after N dative-bonding.

Poster Presentation : **PHYS.P-170**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecular Mechanism Underlying Biomolecular Aggregation

Juyoung Kang, Jinmin Lee, Byeong Hwi Hwang, Sang Hak Lee[*]

Department of Chemistry, Pusan National University, Korea

For a decade, protein aggregation has been considered to be a main cause of several diseases including Alzheimer's disease (AD) and Parkinson's disease (PD). Many researchers have been struggling to understand the molecular mechanism underlying protein aggregation. Up to now, one of the leading theories is that Mg2+ and Ca^{2+} are the two main metal ions that function to create protein aggregates in cells. That being said, there is a very low concentration of metal ions in cells, present only on a micromolar scale. In fact, many millimolar of metal ions are required to induce such protein aggregation. Here, we are interested in finding very small molecules on a millimolar scale that are multivalent, since aggregated proteins are hyper-phosphorylated. Among small molecules in cells, we were interested in the two polyamines spermine and spermidine since they are highly positively charged and exist in high concentration in human cells. Nucleoside triphosphates (NTPs) has three phosphorylated groups that interact electrostatically with polyamines, making them a good model to explain the creation of RNA granules as well as the aggregation of phosphorylated proteins. In this study, we investigated spectral changes of NTPs as a function of polyamine concentration. We found that the absorption band of ATP red-shifted and that of GTP showed a different spectral feature: π - π^* transition red-shifted and n - π^* transition blue-shifted with increasing concentration of polyamines. In addition, we found that a new absorption band of ATP and GTP appeared and evolved over time. This indicates that the aggregates of ATP and GTP grow over time. Thus, we conclude that polyamines are very critical in creating biomolecular aggregates.

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Poster Presentation : **PHYS.P-171**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Water OH stretching frequencies: For 2 dimer geometries

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We obtained 0,1 transition frequencies for two dimers and compared with experimental frequencies. Used theory level in OH potential energy curves is CCSD(T)/CBS limit, and vibrational energy levels from potential curve is obtained by discrete variational representation(DVR) method. In this results, 0,1 frequency errors with experimental values are 5~6cm^{-1}, 1cm^{-1}.

Poster Presentation : **PHYS.P-172**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

The Intraband Transition of Less Toxic Self-Doped Metal Chalcogenide Nanocrystal

Juhee Son, Dongsun Choi[1], Yun Chang Choi[1], Kwang Seob Jeong[1,*]

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

For decades, colloidal quantum dots have been in the spotlight as optical materials due to the tunable bandgap transition. Due to the quantum confinement effect, continuous states within the band are confined to discrete states. Intraband transition occurs between discrete states of the semiconductor nanocrystal. However, due to the fast hot electron relaxation, it had been very difficult to use the intraband transition. In 2014, the steady-state intraband transition in the mid-IR was first reported by Jeong et al. This is a novel result that opens up the possibilities for using the new electron transition of the colloidal semiconductor nanocrystals, particularly in the mid-IR region. Despite the incredible results, there was a concern in dealing with a toxic reagent such as mercury ion compounds. Thus, there has been a demand for replacement with less-toxic materials. In this poster, I will present the optical properties of silver selenide colloidal quantum dots(CQDs) showing the steady-state intraband transition in the mid-IR.In previous studies, Sahu et al. reported that silver selenide CQDs having absorption around 2000 cm-1, but they incorrectly interpreted it as the bandgap transition. Based on our own spectroelectrochemistry and mid-IR emission spectroscopy results, we proved that the mid-IR electronic transition of the silver selenide CQDs arises from the intraband transition. The silver chalcogenides relatively less toxic material will enable many researchers to access to the steady-state intraband transition of the colloidal quantum dot study.

Poster Presentation : **PHYS.P-173**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Femtosecond dynamics from Roussin`s Red Ester with pump wavelength dependence

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Femtosecond infrared spectroscopy was used to study photodissociation dynamics of nitric oxide (NO) from Roussin's Red Ester (RRE), $[Fe2(\mu\text{-}RS)2(NO)4]$ in water in broad time range spanning from 0.3 ps to 10 μs after excitation at various wavelengths (310, 360, and 400 nm). We synthesized $[Fe2(\mu\text{-}N\text{-}acetyl\text{-}cysteine)2(NO)4]$ and $[Fe2(\mu\text{-}N\text{-}acetyl\text{-}penicillamine)2(NO)4]$ which are water soluble and has about 5 times higher thermal stability than $[Fe2(\mu\text{-}cysteine)2(NO)4]$, a previously-known photochemical NO donor. When these RREs were excited, they either release a NO producing a radical species deficient one NO (R), $[Fe2(\mu\text{-}RS)2(NO)3]$ or relax into the ground state without the photodeligation via a metastable state (M). R appears immediately after photoexcitation, suggesting that the photolysis of one NO is faster than 0.3 ps. Some fraction of R geminately recombines with NO on the picosecond time scale (8 – 81 ps) and the remaining R recombines bimolecularly with a rate constant of 3.9 – 25×107 M−1s−1. For a given RRE molecule, the fractional yield of M (0.47 – 0.68) depends on the excitation wavelength (λex) but the relaxation time of M (4.5 – 6.4 ns) was independent of the λex. Although the primary quantum yield (Φ1) of NO photodissociation was found to be 0.32 – 0.53, the final yield for usable NO for other reaction was 0.14 – 0.44 due to the picosecond geminate rebinding (GR) of the dissociated NO with R. Most efficient NO delivery condition was obtained by revealing the λex with lowest GR yield as well as highest Φ1. Detailed photodissociation dynamics of RRE including the NO-producing quantum yield can be utilized in the pin-point usage of NO in chemistry and biology.

Poster Presentation : **PHYS.P-174**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structure and Electrochemical properties of Di-halogenated Aromatic Thiolate Self-assembled Monolayers on Au(111)

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Department of Chemistry, Hanyang University, Korea

Physical and electrochemical properties of metal surfaces can be easily tuned by self-assembled monolayers (SAMs), which are formed by spontaneous adsorption of organic molecules. Especially, SAMs formed from halo-substituted aromatic thiols have been widely studied because of their ability to modify surface energy level, which is useful in electronic applications. Previous studies revealed that properties of the SAMs are significantly affected by packing density and orientation of the adsorbed molecules. However, it is still challenging to obtain high-quality SAMs of aromatic thiols, due to the strong interaction between aromatic backbone and the metal surface, which hampers the lateral interaction between molecules. In our former studies, it was revealed that molecular structures are significantly affected by dipole-dipole intermolecular interaction. In order to examine the dipole-induced organization of halogenated aromatic thiols, we fabricated 2,4-dichlorobenzenethiolate (2,4-DCBT) and 3,4-dichlorobenzenethiolate (3,4-DCBT) SAMs from vapor phase for different time scale. The SAMs were thoroughly characterized by scanning tunneling microscopy (STM) and reductive desorption (RD) method. From our STM results, 2,4-DCBT SAMs showed largely ordered domains with $(2 \times 3\sqrt{3})$ structure, whereas 3,4-DCBT SAMs showed ordered domains with $(\sqrt{3} \times 4\sqrt{5})$ structure. Reductive desorption (RD) results also showed that desorption potential is negatively shifted in both cases as the deposition proceeds.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Simulation Studies on the Anisotropic Effects of Particles by Diffusion

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Department of Chemistry, Dong-A University, Korea

Anisotropic diffusion reactions occurring in natural environments can be implemented using lattice-based Monte Carlo simulations. For example, a complex diffusion reaction system, such as in vivo biological reactions and percolation clusters, can be implemented with a random walk in an irregular lattice. We have found that anisotropy can be efficiently controlled by changing the probability ratio of motion and stay in two- or three-dimensional simulations. By changing the anisotropic effects, we compared results of diffusion influenced reactions. We have also observed changes in the anisotropic effect depending on the initial position. Simulation results are easily obtained and compared in an anisotropic system without theoretical predictions. Theoretical predictions are reproduced in an isotropic diffusion reaction system to confirm the accuracy of the Monte Carlo method.

Poster Presentation : **PHYS.P-176**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Lithium-Ion Battery Solvation Structure study at Low temperature with Cryostat

Yeongseok Chae, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

There are many problems with current lithium-ion batteries that are discharged in unexpected cold due to climate change and in the polar regions. Although many groups are trying to improve the temperature range of LIB, studies have limitations since there is no exact understanding of the molecular level of LIB's solvation system at the low temperature. To break through the current state, we are trying to get information about the change of the solvation structure of LIB at low temperature with a cryostat. We observed that the number of coordinated electrolytes(solvent) increases and the concentration of contact ion pair decreases as the temperature decreases. The number of coordinated electrolytes was calculated through analyzing C=O stretching of them and the trend of the CIP's concentration was confirmed by investigating the P-F stretching of LiPF6(salt). We believe that the temperature dependence of the number of charge carriers has less effect on the temperature dependence of the conductivity than the mobility of charge carriers.

Poster Presentation : **PHYS.P-177**
Physical Chemistry
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Co-doping of Co and Ru into Metallic MoS2 Nanosheets for Overall Water Splitting

Ik Seon Kwon, In Hye Kwak[1], Jaemin Seo, Kim Doyeon, Jong Hyun Lee, Jisun Yoo, Jeunghee Park[*]

Department of Materials Chemistry, Korea University, Korea
[1]*Micro Device Engineering / Microdevices, Korea University, Korea*

Two-dimensional MoS2 nanostructures have recently attracted considerable attention because of their outstanding electrocatalytic properties. In this study, we prepared unique Co/Ru co-doped 1T' phase MoS2 nanosheets that exhibit excellent catalytic activity toward overall water splitting in alkaline solution. The Co atoms were doped homogeneously into MoS2, while a part of the Ru atoms was doped and the rest formed Ru nanoparticles. Co-doping of Co and Ru increased the number of S vacancies/defects and produced more Ru nanoparticles compared to when Co or Ru was doped alone. The excellent catalytic performance of hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) was characterized by low overpotentials of 52 and 308 mV at 10 mA cm-2 and Tafel slopes of 55 and 50 mV dec-1 in 1.0 M KOH, respectively. Analysis of X-ray photoelectron and absorption spectra for the catalysts before/after the electrochemical reactions showed that the MoS2 well-retained its metallic 1T' phase. For HER, the Co/Ru doping sites, as well as the Ru nanoparticles played important roles of dissociating the water and activating the adjacent S sites for the catalytic reduction of H+. The high OER performance was attributed to the efficient production of oxides (CoOOH and RuO2) as the active sites and the maintenance of the high-conductivity 1T' phase MoS2 underneath. This study highlighted the use of multiple dopants to impart bifunctional catalytic activity by optimizing the electronic structures as well as the potential for inexpensive and efficient fuel production.

Poster Presentation : **PHYS.P-178**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Crystal Morphology Observation of Energetic Ink Formulations in Direct-Write Printing Patterns

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The morphology of explosive materials is known to significantly influence the material’s detonation properties, such as their sensitivity to shock and critical dimensions required to sustain detonation. RDX is an organic high-explosive material that been highly utilized for military applications. Significant efforts have been invested in the integration of explosive materials and Micro Electro-Mechanical Systems (MEMS) to make a smart weapon system. An observation in crystal morphology is important to study the miniaturization effect of energetic materials and to know the detonation behavior at small length scales. The aim of this study was to observe and compare the explosive crystal morphology and the patterning of RDX-based composite materials. Formulations of RDX as the explosive material and cellulose acetate butyrate (CAB) as binder were made with two different solvents which were dimethylformamide (DMF) and ɣ-butyrolactone (GBL) and formulations of RDX without binder were made as a comparison. All energetic inks were printed on a silicon wafer substrate with SonoPlot GIX Microplotter and the crystals morphology was analyzed in Scanning Electron Microscope (SEM). With the optimized printing parameters, energetic ink with binder composition showed more connected lines between crystals with tree-like dendrites structure compared to energetic ink without binder that showed small varied-shape crystals with distances and some aggregations. Characterization of printed composites indicated that changes in ink compositions and printing parameters produced various material morphologies.

Poster Presentation : **PHYS.P-179**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Thickness-dependent bandgap and electrical properties of GeP nanosheets

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[3]*Korea University, Korea*

Recently there have been extensive efforts to develop novel two-dimensional (2D) layered structures, owing to their fascinating thickness-dependent optical/electrical properties. Herein, we synthesized thin GeP nanosheets that had a band gap (Eg) of 2.3 eV, which is a dramatic increase from the value in the bulk (0.9 eV) upon exfoliation. This Eg value is close to that of the GeP monolayer predicted by firstprinciples calculations (HSE06 functional). The calculations also indicate a strong dependence of Eg on the number of layers (2.306, 1.660, 1.470, and 1.397 eV for mono-, bi-, tri-, and tetralayers, respectively), and that the band edge positions are suitable for water splitting reactions. Field-effect transistor devices were fabricated using the p-type GeP nanosheets of various thicknesses, and the devices demonstrated a significant decrease in the hole mobility but an increased on–off ratio as the layer number decreased. The larger on–off ratio (104) for the thinner ones is promising for use in novel 2D (photo)electronic nanodevices. Further, liquid-exfoliated GeP nanosheets (thickness ¼ 1–2 nm) deposited on Si nanowire arrays can function as a promising photoanode for solar-driven water-splitting photoelectrochemical(PEC) cells. Based on the calculated band offset with respect to the Fermi levels for the two halfreactions in the water splitting reaction, the performance of the PEC cell can be explained by the formation of an effective p-GeP/n-Si heterojunction.

Poster Presentation : **PHYS.P-180**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

NiS$_x$ Nanocrystals on Si Nanowire Array Photocathodes for Solar-Driven Hydrogen Production

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Photoelectrochemical water splitting has recently attracted much attention because of a promising technology for generating clean and renewable hydrogen energy. Herein, we report NiS and NiS$_{1.97}$ nanocrystals (NCs) as excellent catalysts for photoelectrochemical hydrogen production. Photoelectrodes were fabricated by growing the NiS and NiS$_{1.97}$ NCs directly onto Si nanowire (NW) arrays for Si-based photoelectrochemical (PEC) cells. The controlled synthesis of free-standing NiS and NiS$_{1.97}$ NCs was also achieved by the sulfurization of nickel hydroxide nanosheets. . For Si NW photocathode, the deposited NiS NCs enhanced the performance of solar-driven water-splitting PEC cells, by increasing the photocurrents and shifting the onset potentials, which is more significant than the NiS$_{1.97}$ NCs. The NiS NCs exhibited the higher performance than NiS$_{1.97}$ NCs for electrocatalytic hydrogen evolution.Detailed structure analysis using X-ray photoelectron spectroscopy and X-absorption near edge fine structure reveals that the NiS is more metallic than the NiS$_{1.97}$ and retain the crystal phase during the hydrogen evolution. These factors would play an important role in increasing the catalytic activity toward both hydrogen evolution reactions.

Poster Presentation : **PHYS.P-181**
Physical Chemistry
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Two-Dimensional MoS_2-Melamine Hybrid Nanostructures for Enhanced Catalytic Hydrogen Evolution Reaction

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Two-dimensional (2D) MoS2 nanostructures have attracted much attention in recent years because of their excellent electrocatalytic activity toward the hydrogen evolution reaction (HER). Herein, we report unique 2D hybrid nanostructures of MoS2 and melamine synthesized via a one-step solvothermal process. Few-layered metallic 1T’ phase MoS2 nanoflakes were anchored homogeneously on the nanoplatelets composed of orthorhombic phase melamine. At a controlled concentration, the melamine molecules also intercalated into the 1T’ phase MoS2 by forming charge-transfer complexes. The hybrid complexes with 7% intercalated melamine exhibited excellent performance for catalytic HER, with a current of 10 mA cm-2 at 0.136 V (vs. RHE) and a Tafel slope of 37 mV dec-1. First-principles calculations showed that the intercalation of hydrogen-bonded melamine clusters could stabilize the 1T’ phase MoS2 via substantial charge transfer. The activation barrier was calculated for the Volmer-Heyrovsky reactions, by identifying the active sites of Volmer reaction as the basal S atoms above the hydrogen-bonded amine group of melamine. This rationalizes the dependence of catalytic activity on the concentration of intercalated melamine. The present study highlights the opportunities of producing unique 2D hybrid complexes to enhance the HER catalytic activity by controlling the intercalating organic molecules.

Poster Presentation : **PHYS.P-182**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Two-Dimensional Ternary Composition Layered Structures with Wide Direct Band Gap

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The recent discovery of graphene has given rise to significant an 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 the remarkable properties of the 2D nanostructures is their unique band gap increase at the 2D limit by quantum confinement effects. As new potential class of 2D materials, MPSx compounds (M = Ga, Bi, Sn, B, Cr ; x = 3-4) have been recently proposed from theoretical calculations. In the present work, we synthesized that two-dimensional layered gallium thiophosphate (GaPS4) using the exfoliation of bulk crystals that were synthesized by Bridgeman melt-growth method. According to the previous theoretical works, the Eg of their monolayer can reach 3.55 eV, whereas that of the bulk is below 2.38 eV. The exfoliation into thin nanosheet revealed the dramatic increase of the optical band gap, which is in the ultraviolet visible-light range of 3.55-2.38 eV.

Poster Presentation : **PHYS.P-183**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Scanning Transmission Electron Microscopy of Transition Metal dichalcogenide Nanosheets

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[3]*Korea University, Korea*

Two-dimensional layered structures have recently drawn worldwide attention because of their intriguing optical, electrical, and catalytic properties. Molybdenum selenide (MoSe2) is considered as the most promising catalysts for water-splitting hydrogen evolution reaction to replace the expensive Pt. MoSe2 exhibits polymorphic phases such as stable semiconducting 2H (trigonal prismatic) phase, metastable metallic 1T phase, and metastable 1T' (distorted 1T) semi-metallic phase, depending on the synthesis procedure. Many strategies have been developed to maintain the metastable 1T and 1T’ phases by controlling its electronic structures. We found that the control of Mo/Se ratio is a promising strategy to enhance the stability of 1T and 1T’ phase and their HER performance. To directly observe the polymorphic phases, high-angle annular dark-field scanning (HAADF) in an advanced (spherical) aberration-corrected high-resolution scanning resolution transmission electron microscopy (STEM) was employed. The HAADF STEM image recognizes the Mo and Se atoms in precise position, providing the atomic arrangements of polymorphic phases.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

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Theoretical Study on Hazardous Gas Adsorption Structure and Adsorption Energy Using Germanin SheetGermanene Sheet

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The air pollution problem caused by sediment and yellow dust has become a big issue in recent years at home and abroad. Such air pollution is known to be caused by the continuous use of fossil fuels, such as factory and automobile exhaust. Graphene or similar graphene sheets, which have been actively researched recently, are expected to be used as gas sensors capable of confirming the presence of these harmful gases(COx, NOx, SOx). In this study, the structural characteristics and binding energy of these toxic gases adsorbed on germanium($Ge_{32}H_{14}$) sheet were presented using density functional theory(DFT).The molecular structure was optimized at the B3LYP/CC-pVDZ and CAM-B3LYP/CC-pVDZ theory levels, and the vibration frequency was calculated to identify the thermodynamic most stable molecular structure.The binding energy was calculated from the point energy at the MP2/CC-pVDZ theory level and the zero vibration energy(ZPVE) was corrected. Gas adsorption to Germanene was predicted that COx, NOx and the like will undergo physical adsorption and SOx to chemisorption.

Poster Presentation : **PHYS.P-185**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

A field-portable GC for trace detection of volatile organic compounds in air samples

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Current study describes a portable GC (36×26×15 cm^3, 5.5 kg) for real-time monitoring of trace gas mixture in air sample. This system is comprised of a CNT sponge preconcentrator, a low thermal mass column module with capillary column, an electronic pneumatic control of filtered ambient air as a carrier gas, and a home-built photo ionization detector. The relative standard deviation of retention time and peak intensity variation during 10 hours operation showed < 0.21% ad < 1.0%, respectively, demonstrating a good reproducibility for continuous measurements. Sensitivity increase of 100-fold by preconcentrating an adsorption volume of just 90mL results in the improved detection limit, typically in the sub-ppb range. The results show that this portable GC can be widely applied to the on-site detection, including indoor air quality, industrial emission control, rapid detection of explosives in public place, breath analysis, environmental monitoring, chemical processes, and regulation of contaminant emission

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Generation of broadband Near-Ultra-Violet (NUV) source

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Since broadband laser source can provide wide excitation spectrum, which can increase the dynamic range of impulsive vibration spectrum in Fourier domain, it has been widely used especially in pump-probe spectroscopy. Although necessity of simpler and wider laser source was raised from time to time, it is hard to enhance the quality of laser source using conventional method. For this reason, we studied about a new method of fabricating a broadband NUV laser source. Generating the broadband NUV laser was simulated and its results were compared with the experiments. Comparing with the conventional method, we can obtain simpler and wider spectral bandwidth.

Poster Presentation : **PHYS.P-187**
Physical Chemistry
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Theoretical and experimental branching ratio about ternary cluster cations

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In our previous study, we measured the branching ratios about dissociation of two solvent molecules in six ternary cluster cations, aniline-water-ethanol cation (AWE+), aniline-water-isopropanol cation (AWP+), aniline-methanol-ethanol cation (AME+), aniline-water-methanol cation (AWM+), aniline-water-pyrrole cation (AWPy+), and aniline-water-benzene cation (AWB+). We tried to explain the branching ratios theoretically using the phase space theory (PST) because the dissociation of solvent molecules occurred through loose transition states (TS) which did not have any barriers of reverse reaction. In the PST, an orbiting transition state (OTS) located at the maximum of the long range effective potential was assumed and the rotational constant and vibrational frequencies of the products were used in the rate constant calculations. However, the OTS/PST calculations could not explain the experimental branching ratios. Although it was hard to apply the conventional Rice-Ramsperger-Kassel-Marcus (RRKM) theory on ternary cluster cation because of loose TS, we could predict the experimental result with RRKM theory applying simple assumption.

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Physical Chemistry
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Physical Properties of Self-Doped Colloidal Quantum Dots and Tellurium Element

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The researches of colloidal quantum dots (CQDs) focused on the bandgap transition for decades. The recent research has substantiated that the self-doping property leads the intraband transition in the nanocrystal. In this poster, I will present the mid-IR photoluminescence(PL) and magnetism of self-doped $Cd_xHg_{1-x}Se$ alloy and Ag2Se nanocrystals. Also, strong mid-IR photoluminescence and lasing from the tellurium element.The CdHgSe alloy nanocrystals have the electronic transition progressively shift from visible to the mid-IR localized surface plasmon resonance (LSPR) by increasing the quantity of mercury substitution in the CdSe nanocrystals. The increment of the mercury ratio in the alloy changes the major transition to the mid-IR region and successfully measured the mid-IR PL with the home-built mid-infrared spectrometer. Surprisingly, the mid-IR emissive alloy nanocrystal showed singly-occupied quantum-state from the EPR measurement, and free-electron signal as the LSPR revelation, respectively. The mid-IR PL from the Ag2Se self-doped CQDs is measured with the home-built spectrometer and revealed that the electronic transition in the mid-IR region is indeed the intraband transition. Surprisingly, strong mid-IR PL and lasing are observed from the tellurium element. The annealing procedure germinates micrometer size tellurium crystal, and interestingly, blue-shifted the PL peak position. Further cryo-temperature study of microcrystal tellurium showed a lasing emission. The tellurium material could be a standard mid-IR PL illuminant in further study.

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

The Structural Origin of the Electron Affinity of Poly-Aromatic Hydrocarbon

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Poly-Aromatic Hydrocarbon (PAH) molecules are building blocks for graphene. It is important to understand the basic molecular properties of PAH molecules, in particular electron affinity and ionization energy, in order to determine the electrical property of graphene. In this study, we theoretically investigate the electron affinity of PAH molecules using density functional theory (DFT). We know that anthracene and phenanthrene have different electron affinities (0.53 eV and 0.13 eV, respectively), even though they have the exact same molecular formula. This is because when butadiene is added to the naphthalene molecule in each of the two compounds, the butadiene assumes a different molecular reaction position as it adds a benzene ring. Examining this further, e found the general principle governing the electron affinity of PAH molecules as a function of the different structure and number of benzene rings.

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Poster Presentation : **PHYS.P-190**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecular-Scale STM Observation on the Formation of Self-Assembled Monolayers on Au(111) Derived from Aromatic Selenocyanates

Seul-ki Han, Jaegeun Noh*

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Aromatic selenolate self-assembled monolayers (SAMs) have received great attention because of their chemical stability higher than that of aromatic thiol SAMs and their attractive potential applications such as molecular electronics, charge transfer, and biosensor. Also, addition of methylene unit between the phenyl group and the headgroup is an effective way to control packing density of SAMs on gold or silver substrate. In this study, to understand the formation and structure of the SAM derived from aromatic selenocyanates, we investigated the SAMs of phenyl selenocyanate (PhSe-CN), benzyl selenocyanate (BnSe-CN), 2-phenylethyl selenocyanate (2-PhESe-CN), 3-phenylpropyl selenocyanate (3-PhPSe-CN), and 4-phenylbutyl selenocyanate (4-PhBSe-CN) on Au(111) by scanning tunneling microscopy (STM), contact angle (CA), cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS). XPS result indicates that aromatic selenolate SAMs were formed via cleavage of Se-CN bond from Ph(CH$_2$)nSe-CN (n = 0-4). STM investigation shows that the formation and structure of aromatic selenocyanate SAMs on Au(111) were influenced by the number of methylene spacer. The 2-PhSe SAMs on Au(111) showed a $(\sqrt{3} \times \sqrt{19})$ structure with higher packing density than that of the BnSe SAMs on Au(111) with a $(\sqrt{3} \times 3\sqrt{3})$ packing structure. In addition, 3-PhPSe SAMs on Au(111) have a $(\sqrt{3} \times \sqrt{3})$ structure. CV measurement showed reductive desorption potential was shifted to negative direction with increasing the number of methylene spacer of aromatic selenolate SAMs, which is good consistent with STM observations.

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Poster Presentation : **PHYS.P-191**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Quantum chemical dynamics of the dissociative electron attachment to SF_5-X:Cl, Br, F, C_2H_3, C_6H_5, CF_3 and SF_5

Hyoung-Chul Ham, Kyoung-Koo Baeck*

Department of Chemistry, Gangneung-Wonju National University, Korea

SF_5-X (X=Cl, Br, F, C_2H_3, C_6H_5, CF_3, SF_5) have been the targets of many theoretical and experimental studies because of their global warming effects. The dissociative electron attachment to the parent molecules seems to be the most probable removal process in natural environment. Though many thermochemical and kinetics study on the processes were conducted so far, microscopically detailed dynamical study of their early-time stages is still quite limited. With basic quantum chemical studies on the stationary structure, vibration properties, bond dissociation energy, electron affinity of the parent compounds and all possible their neutral and anionic fragments, we carried out ab initio molecular dynamics (AIMD) studies on the early time dissociation stages. Somewhat unique features of SF_5-C_2H_3 and SF_5-CF_3, in compare with others, were disclosed, and main emphases of our discussion will be placed on the early-time dynamics of SF_5-C_2H_3 and SF_5-CF_3 systems.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Interpretation of Hofmeister series: Formation of an amide tautomer by divalent cations

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Ion-specific effects on peptides and proteins are crucial to the biomolecular structure. Compared with the significant role of anions, the subtle effects of cations on proteins have not been clearly understood. Importantly, divalent cations like Ca2+ and Mg2+ are known to be crucial to biological functions. Herein, we report that the direct binding of the divalent cations to the amide oxygen in aqueous solution triggers an amide–iminolate tautomer equilibrium. For N-methyl acetamaide (NMA) dissolved in aqueous 5M CaCl2 solution, the formation of an amide tautomer is strongly supported by two-dimensional infrared (2D IR) spectroscopy of the amide vibration and molecular dynamics (MD) simulations of molecular phenomenon. The interconversion timescale (~17 ps) between the tautomers confirms that Ca2+ forms direct contact with the amide O intermittently. These results confirm the arrest of an unusual amide tautomer by the divalent cations and provide an explanation for the shift in the aggregation pathway of neurotoxic peptides in the presence of divalent cations.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

The Effect of the *ortho* Nitro Group in the Solvolysis of Benzyl and Benzoyl Halides

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A kinetic study was carried out on the solvolysis of *o*-nitrobenzyl bromide (**1**) and *p*-nitrobenzyl bromide (**3**), and *o*-nitrobenzoyl chloride (**2**) in a wide range of solvents under various temperatures. In all of the solvents without aqueous fluoroalcohol, the reactions of **1** were solvolyzed at a similar rate to those observed for **3**, and the reaction rates of **2** were about ten times slower than those of the previously studied *p*-nitrobenzoyl chloride (**4**). For solvolysis in aqueous fluoroalcohol, the reactivity of **2** was kinetically more reactive than **4**. The *l*/*m* values of the extended Grunwald–Winstein (G–W) equation for solvolysis of **1** and **2** in solvents without fluoroalcohol content are all significantly larger than unity while those in all the fluoroalcohol solvents are less than unity. The role of the *ortho*-nitro group as an intramolecular nucleophilic assistant (internal nucleophile) in the solvolytic reaction of **1** and **2** was discussed. The results are also compared with those reported earlier for *o*-carbomethoxybenzyl bromide and *o*-nitrobenzyl *p*-toluenesulfonate. From the product studies and the activation parameters for solvolyses of **1** and **2** in several organic hydroxylic solvents, mechanistic conclusions are drawn.

Poster Presentation : **PHYS.P-194**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Identification of CPN-mediated Glutamate transport mechanisms upon its ionic charged status

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Lipid bilayers play many roles in the cell. They act as a physical barrier to protect the interior of the cell from its environment. They also play as a communication platform between the cytoplasmic region and the extracellular space. Because these functions of lipid bilayers are mostly mediated by membrane proteins, there has been many attempts to imitate membrane proteins. Among these attempts, cyclic peptide nanotubes(CPNs) have a high biocompatibility and induce translocation of molecules across the lipid bilayer. Many studies have shown that ions and some kinds of small hydrophilic molecules like glucose can penetrate across the lipid bilayer through CPNs, but most of them focused only on non-charged hydrophilic molecules. In this study, we investigate the dependence of the energetics and dynamics of transport of glutamic acid (GLU) through CPNs on its charged state. We conducted a series of MD simulations for GLU with different charges (-1, 0, +1) and 8x cyclo[-(D-Leu-Trp)4-] CPN and calculated potential of mean force (PMF) profiles and position-dependent diffusion coefficients. The simulation results show that negatively charged GLU, which is largely abundant at physiological pH, has the highest energy barrier that makes the permeation coefficient of the negatively charged GLU very small. Zero charged form of GLU has a lower energy barrier, implying that the electrically neutral GLU pass through CPNs more easily than negatively charged form. The PMF profile for positively charged form of GLU shows a global energy well of -15 kcal/mol instead of energy barriers, indicating that CPNs are designed to be cation-selective. Our observations suggest that transport of GLU through CPNs is dependent on its charged status owing to the cation-selective nature of CPNs.

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Poster Presentation : **PHYS.P-195**
Physical Chemistry
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A DFT Study on the Mechanism of Lithium Halides Catalyzed Hydroboration of Aldehydes with Pinacolborane

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Hydroboration is an important and fundamental reaction system in organic chemistry for the reduction of unsaturated, carbonyl compounds. On the basis of the experimental results, computational studies were carried out to explore a mechanistic understanding of the lithium halides catalyzed hydroboration of aldehydes with pinacolborane (HBpin). From the DFT study, the lithium halides catalyzed hydroboration of aldehydes with HBpin occur through the catalytic cycle of a hexagonal ring transition state and ligand exchange reactions. Further, we studied how halide species affect the reaction mechanism. Finally, the possible mechanism was proposed by integrating the experimental and computational results.

Poster Presentation : **PHYS.P-196**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fluorescence spectroscopic investigation of the interaction of cationic surfactants with water-soluble polymers in aqueous solution

Hyomin Kim, Han Gook Cho*, Byeong-Seo Cheong*

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The interaction of cationic surfactants, alkyltrimethylammonium bromide with uncharged, water-soluble polymers, poly(vinyl alcohol) and polyvinylpyrrolidone, in aqueous solution was studied by fluorescence spectroscopy using several different fluorescence probes. The fluorescence probes exhibited changes in emission intensity and/or wavelength as the concentration of the surfactant increased in the polymer-surfactant solution, reflecting the change in microenvironment surrounding the fluorescence probe. In particular, the excited-state proton transfer of pyranine, a photoacid, was found to be very sensitive to the interaction between polymer and surfactant. The effects of varying the concentration and molecular weight of polymers and the chain length of surfactant were investigated to gain insight into the polymer/surfactant interaction. Based on the spectral variations observed and conductivity measurements, the interaction model between polymer and surfactant was proposed.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Solvent effects on the Raman spectra of p-nitroaniline, N,N-dimethyl-p-nitroaniline, and p-nitropheol in solution

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Raman spectra of p-nitroaniline, N,N-dimethyl-p-nitroaniline, and p-nitropheol were measured in various solvents as well as in the solid state, particular attention being paid to the shift in Raman bands caused by solvents. Among the Raman bands observed, the shift in NO2 stretching band, which all molecules have in common, was found to be very solvent-dependent. The change in band shape of NO2 stretching band was also observed depending on the solvent. The Raman shifts in various solvents were compared to the solvatochromic shifts observed in the UV/Vis spectra. In order to understand the solvent-dependent Raman shifts and to aid the spectral assignment, density functional theory (DFT) calculations were performed with inclusion of solvent effects. Possible interactions of NO2 group with solvents were discussed on the basis of the observed spectra and the DFT results.

Poster Presentation : **PHYS.P-198**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Excited-state proton transfer of 7-hydroxy-4-methylcoumain in reverse micelles composed of various water-organic solvents by fluorescence spectroscopy

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

The excited-state proton transfer (ESPT) reactions of 7-hydroxy-4-methylcoumain(7H4MC) were studied in AOT and BDHC reverse micelles prepared with mixed solutions of water and several different polar organic solvents. The degree of ESPT was estimated by observing the fluorescence emission bands originating from the excited neutral, anionic, and tautomeric forms of 7H4MC. The fluorescence intensity ratios among the three emission bands were measured and compared between regular reverse micelles and the reverse micelles composed of water-organic solvent. We particularly noticed different ESPT behavior as the mole fraction of organic solvent changes in reverse micelles, compared to the case of bulk solutions of water-organic solvent. The observed behavior was discussed in terms of possible configuration and interaction of 7H4MC in aqueous organic solution pool in the reverse micelles.

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Poster Presentation : **PHYS.P-199**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Direct Evidence of Channel-Water Dynamics Related with the Structure Changes in a Transmembrane Ion Channel

Jin Gyu Seol, Hyejin Kwon, Yung sam Kim*

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Knowledge of both structural and dynamical characteristics are essential to understand the function of membrane proteins. Two-dimensional infrared (2D IR) spectroscopy can detect small changes in secondary structure as well as measure fast structure dynamics on the picosecond timescale. Here, we report a 2D IR spectroscopic investigation to probe the backbone configurations of the transmembrane domain of M2 proton channel in a solid-supported membrane environment. Our results show that a helix kink at higher pH (7.5) occludes the passage of water molecules into the channel, making the channel inactive. A conformational change upon lowering the pH (5.5), shows ultrafast hydrogen-bond dynamics between the amide carbonyls of the transmembrane protein and the water molecules, confirming the presence of water inside the channel in the active state. This result suggests that the rate of proton diffusion is closely related to the water dynamics induced by the structural change in the protein.

Poster Presentation : **PHYS.P-200**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecular Engineering of Two Manager and Host Iridium Dopants and Triplet Energy Transfer between them for Improvement and Optimization of Blue PHOLED Device Performance

Jin-Hyoung Kim, Bo-Sun Yun, Jeong-Wan Yu, Su-Jin Kwak, Chul Hoon Kim*, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In this study, we prepared phenylimidazole-based C^N-cyclometalated Ir(III) complexes (**DMP**, **TPF2**) and C^C-cyclometalated Ir(III) complex (**PMP**), and investigated the energy transfer process by examining the intermolecular interactions between the two cyclometalated Ir(III) complexes. In films doped with 3% $Ir(C^{\wedge}C)_3$ complex (**PMP**) and 15% $Ir(C^{\wedge}N)_3$ complex (**DMP** or **TPF2**), the **PMP** effectively induced energy transfer to the **DMP** or **TPF2**. This intermolecular energy transfer process was investigated using a picosecond time-resolved emission spectroscopic method. In the case of mixing **PMP** with **DMP**, where two types of luminescence were observed at 470 nm and 580 nm, the emission at 470 nm was due to **DMP**, while the emission at 580 nm can be assigned as the intermolecular exciplex emission. By contrast, in the case of mixing **PMP** with **TPF2**, the emission at 465 nm corresponding to the **PMP** emission region decreased for 18.5 ns, while the emission at 530 nm corresponding to **TPF2** increased. This emission can be attributed to the energy transfer from **PMP** to **TPF2**. In addition, no change was observed in the longer wavelength region than the **TPF2** emission region for 10 μs. We analyzed the energy transfer process when **PMP** was added to the dopant (**DMP** and **TPF2**) and found that **TPF2** was more efficient than **DMP** in the device without **PMP** doping, but it showed performance deterioration in high current density (>1 mA/cm^2) owing to activation of fluorinated ligands. Finally, it was confirmed that the operation lifetime and efficiency of the device were improved by doping 3% of **PMP** in emissive layer (EML).

Poster Presentation : **PHYS.P-201**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of piperidine: Determination of accurate ionization energy and conformation structure

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[1]*New and Renewable Energy Research Center, Ewha Womans University, Korea*

Piperidine, which is a saturated six-membered heterocyclic compound possessing a nitrogen atom, has been paid much attention to the conformational structure in the electronic state governed by the highest occupied molecular orbital (HOMO), which determines the ring-puckering potentials associated with the N-inversion motion. We measured the high-resolution vibrational spectra of piperidine cation in the ground electronic state under various molecular beam conditions utilizing the conformer-specific vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy, from which the accurate ionization energy was determined to be 64,473 ± 3 cm^{-1} (7.9936 ± 0.0004 eV). The measured VUV-MATI spectra could be analyzed by the Franck-Condon (FC) simulations, based on the optimized structures in the S_0 and the D_0 states at the density functional theory levels. Consequently, it was found that the equatorial conformer is more stable than the axial conformer in the S_0 state, while only axial conformation similar to the axial conformer permits in the D_0 state due to removal of a lone pair electron from nonbonding orbital of the nitrogen atom in piperidine upon ionization. It implies that upon ionization, the equatorial conformer prefers the FC favorable transitions such as the ring-puckering vibrational mode, but the 0-0 band of the axial conformer would be the most intense among all transitions associated with axial conformer, showing entirely small intensities due to low population in the S_0 state.

Poster Presentation : **PHYS.P-202**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Conformational study of the neutral and the cationic 3,4-dihydro-2H-pyran by conformation-specific VUV MATI spectroscopy

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It has been known that 3,4-dihydro-2H-pyran (34DHP), which is the pseudo five-membered heterocyclic compound with unsaturation adjacent to oxygen atom, has two conformations in the neutral ground state, where the half-chair form is more stable than the boat one. In order to investigate the conformational stability in the cationic state, we measured the high-resolution vibrational spectra of 34DHP cation in the ground electronic state under various molecular beam conditions utilizing the conformer-specific vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy, from which the accurate ionization energy was determined to be 8.3355 ± 0.0004 eV (67,230 ± 3 cm^{-1}). The measured VUV-MATI spectra could be analyzed by the Franck-Condon (FC) simulations, based on the optimized structures in the S_0 and the D_0 states at the density functional theory levels. The details on the conformational stability of 34DHP will be discussed in the poster.

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Molecular Self Assembly of Dimethyl Disulfide and Dimethyl Trisulfide on Au(111)

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Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are organic thin films formed by spontaneous adsorption of thiol molecules, which have specific affinity to the coinage metal substrates. Although the thiols are most common head group for the SAMs, several studies have employed disulfides as alternatives to thiols in order to understand the binding mechanism of sulfur head groups. Especially, dimethyl disulfide is suitable for studying the effect of the head groups, since they have the shortest alkyl chain, which minimizes the influence of lateral interaction. To better understand the effect of head groups on the formation of the SAMs, we compared the SAMs formed from disulfides and trisulfides with one more sulfur atom. The resulting SAMs were investigated by scanning tunneling microscopy (STM) and cyclic voltammetry (CV) while changing immersion time. Our STM images revealed that dimethyl trisulfide SAMs were less ordered than dimethyl disulfide SAMs at same immersion time. CV measurement showed that reductive desorption potential of dimethyl disulfide SAMs appeared to be single peak at -730 mV regardless of immersion time. On the other hand, dimethyl trisulfide SAMs formed for 10 min showed no peak and those formed for 1 h showed three peak at -910 mV, -990 mV and -1090 mV, respectively.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Dual frequency comb vibrational optical activity spectroscopy

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It is of great importance to develop techniques to measure optical activity when we investigate biomolecules. Since CD is a extremely weak value, time-resolved CD spectroscopy is experimentally challenging. Here, we demonstrated that it is possible to measure electronic optical activity free-induction-decay (OA-FID) field of tris-(enthylenediamine)3 chloride with dual frequency-comb(DFC). We utilized two phase-locked mode lock lasers whose center frequency is 3100 nm and repetition rate is detuned in slightly different frequency. By measuring parallel FID field in time domain and transforming the measured quantities in time domain into frequency domain via fast Fourier transform by DFC, the complex susceptibility can be obtained, whose imaginary parts and real parts are related to circular dichroism(CD) and optical rotation dispersion(ORD), respectively. By DFC, OA-FID can be measured with simple instrumentation and high data acquisition speed. We anticipate that time-resolved CD spectroscopy with DFC can bring tremendous advantages to the dynamic studies of optically active molecules.

Poster Presentation : **PHYS.P-205**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structure Studies of Poly(3-hexylthiophene-2,5-diyl) (P3HT) Using Femtosecond Stimulated Raman Spectroscopies

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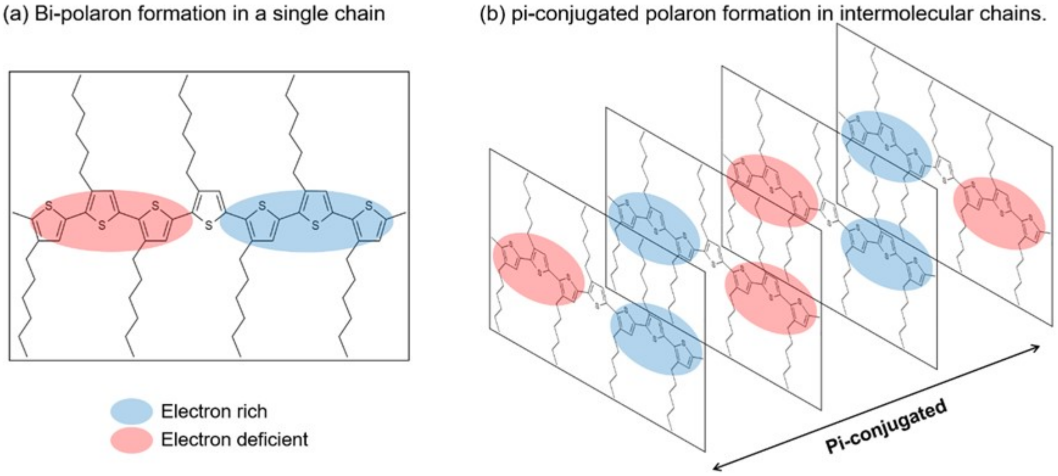
Highly pi-conjugated poly(3-hexylthiophene) (P3HT) shows an effective formation of polaron, which is critical in organic photovoltaic performance. In our theoretical and experimental studies, this polaron generation can be stimulated by a highly oscillating vibrational motion of C=C. We exploited excited-state femtosecond stimulated Raman spectroscopy (FSRS) and found the two prominent Raman peaks at ~1450 cm$_{-1}$(C=C stretching) and 1350 cm$_{-1}$ (C-C stretching) which are ~20 cm$_{-1}$ red-shifted from ground-state Raman peak locations. This red-shift dynamics is a pure excited-state reaction which occurs within 5 picoseconds after the excitation. Using density functional theory, we have correlated the redshifts to asymmetric or half-symmetric C=C and C-C stretches, not the entire symmetric stretching modes vibrating along the whole chain. Additionally, we also have found the elongated C=C motion can effectively increase the electron density localization and shortened C=C does vice versa. Thus, this motion can effectively initiate the formation of intramolecular polarons, supporting that the nuclear wave packet motions and electron densities are strongly correlated in P3HT. In addition, we have studied vibrational Raman modes and depolarization ratios of annealed and non-annealed P3HT films to account for the structural dependence on intermolecular interactions.


(a) Bi-polaron formation in a single chain

(b) pi-conjugated polaron formation in intermolecular chains.

Poster Presentation : **PHYS.P-206**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Quantitative study of mammalian gene expression based on chromatin looping structure

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In mammalian cells, actively transcribed genes are organized to be in close proximity to each other, forming transcriptional interactome. For genes belonging to an interactome, their expressions are highly correlated in a positive sense. In addition, it has been recently found that transient or stable aggregates of RNA polymerase (RNAP) II molecules are formed around such interactomes. Understanding how mammalian gene expression is influenced by such factors Is still missing. In order to provide an analytical framework targeting this problem, we present the mammalian gene expression model with RNAP II cluster dynamics and gene activity fluctuation taken into account. From the RNA-sequence experimental data over five human breast cancer cell lines, we could extract the correlation-noise relationship for genes transcribed through basal promoters and multi-gene interactomes. It is shown that the present theory can make a quantitative prediction to the experimental result in conjunction with three different degradation models

Poster Presentation : **PHYS.P-207**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Lattice-Based Monte Carlo Simulation Studies on Lattice Constant Effects in the Diffusion-Influenced Reaction

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The random walk simulation usually predicts the theoretical results in the diffusion-influenced reaction field with accuracy in various dimensions. While one dimensional results of simulation and theoretical approaches are in perfect agreement, significant differences are observed between simulation and theoretical results in two and three dimensions. We have quantified the difference rigorously. We study why the differences exist in higher dimensional results and suggest the optimum lattice constants.

Poster Presentation : **PHYS.P-208**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Electrochemical Reduction of CO_2 on Gold Nanoparticles-Reduced Graphene Oxide Modified Electrode

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

Due to its excellent thermal/electrical conductivity, great chemical stability, and high surface area, graphene has been known as catalyst support with remarkable performance. Therefore, there has been many attempts to prepare graphene-based composites as catalytic materials in order to exploit specific advantages of graphene. In this work, reduced graphene oxide (rGO)-based composites with gold nanoparticles (AuNPs) were synthesized and used as catalysts for the electrochemical reduction of carbon dioxide (CO_2). The AuNPs/rGO composites were prepared through conjunction of positively charged AuNPs and negatively charged rGO nanosheets. The as-prepared nanocomposites were investigated using various methods including transmission electron microscopy, scanning electron microscopy, powder X-ray diffraction, and UV-vis spectroscopy. AuNPs/rGO nanocomposites showed greatly improved resistance against oxidation and aggregation, and also AuNPs/rGO-modified electrodes displayed excellent catalytic activity towards the electrochemical reduction of CO_2, due to the high specific surface of rGO and great catalytic effect of AuNPs.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Folding Ability of Telomeric Human G-quadruplex Structures: Using Fluctuating Thermodynamic Methods

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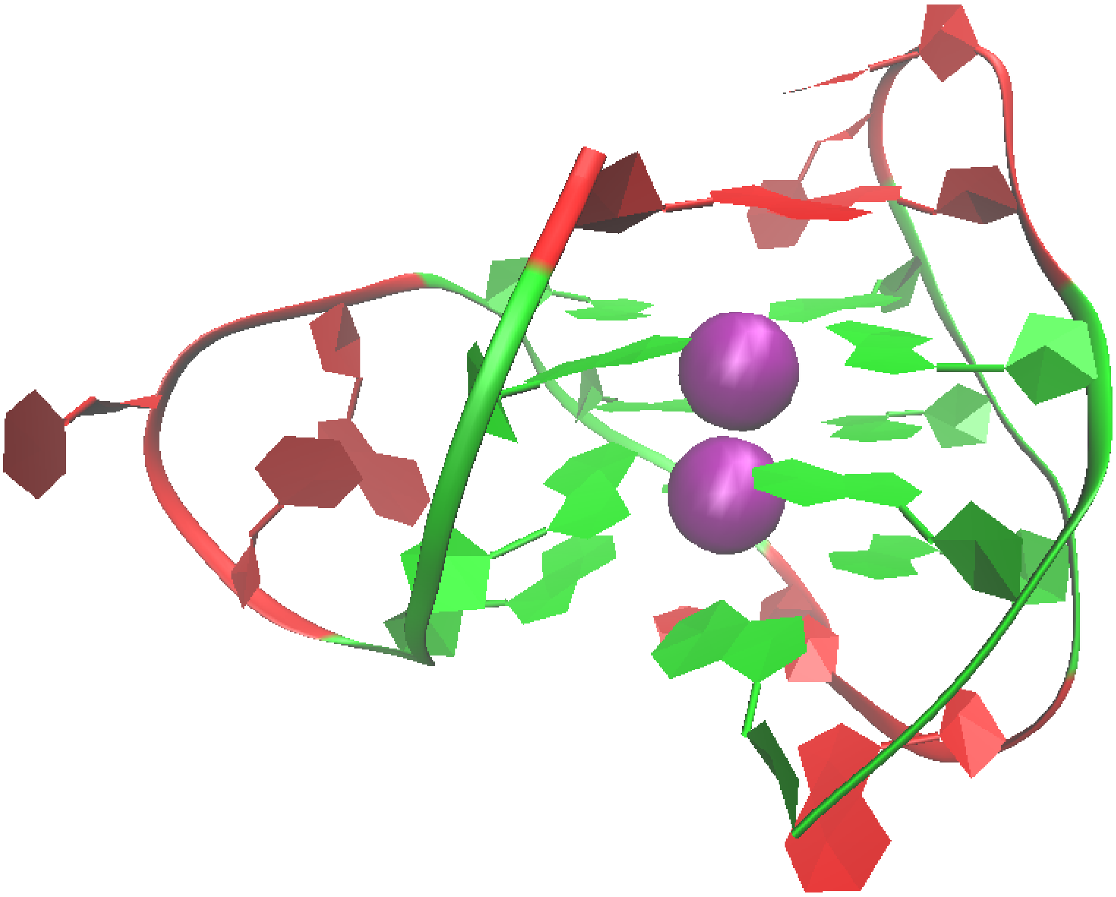
G-quadruplex is the DNA complex consisted of the telomere with ligands, which is located at the end of genomic sequences in chromosomes. Its genomic instability causes serious problems of transcription and translation, such as the production of cancer cells. In this study, we performed molecular dynamics simulations of microsecond time-scale for three types of telomeric human G-quadruplex (Tel22), called antiparallel, hybrid and parallel. Also, we computed thermodynamic parameters including conformational entropy by using fluctuating thermodynamic methods. We find that the hybrid type of G-quadruplex exhibits the highest conformational entropy among the three. Based on the conformational and thermodynamic analyses, we provide the molecular origin of the DNA thermodynamic instability and its consequence to the DNA folding ability.



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Poster Presentation : **PHYS.P-210**
Physical Chemistry
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ProWaVE: Web-based Computational Platform for Protein Solvation Free Energy

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Solvation free energy of a protein is a key thermodynamic quantity in modulating protein interactions, such as protein-ligand interactions, protein assembly, and protein aggregation. Computing protein solvation free energy is not trivial due to the complicated parameter settings and computational time. Protein surrounding Water Visualization and Energetics (ProWaVE) provides a web-based computational platform with simplified and automated steps for the protein data bank (PDB) file processing and computational resources for calculating solvation free energy using fluctuating thermodynamics technology. ProWaVE also supports the decomposition of the solvation free energy into its components, i.e. solvation enthalpy and solvation entropy as well as its residual solvation free energy decomposition with user-friendly interfaces. The development of the ProWaVE web platform is still ongoing. ProWaVE will continue to help researchers in bio science fields, especially those who wants to understand protein-water interactions.

Poster Presentation : **PHYS.P-211**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Pulse Electrodeposition of Silver Nanoparticles on Carbon Paper Electrode for Non-Enzymatic Electrochemical Detection of Nitric Oxide

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A general approach for improving the performance of a catalyst without changing the properties of the material is to adjust its morphological structure to have a large surface area and high catalytic activity. The hierarchical 3-D catalysts with large surface area and good activity can be produced when incorporated into gas diffusion electrodes (i.e., carbon paper). In this study, silver nanoparticles (AgNPs) were directly deposited on carbon paper (CP) for the non-enzymatic detection of nitric oxide ions using pulse electrodeposition and sonication techniques. The application of sonication and potentiostatic pulse deposition can improve the mass transfer of Ag ions from the bulk into the surface of CP electrode. The deposition characteristics of AgNPs on CP were investigated by using scanning electron microscopy, X-ray photoelectron spectroscopy, and powder X-ray diffraction. Due to the large surface area of CP and high catalytic activity of AgNPs, nitric oxide (NO) ions could be detected with high sensitivity using an amperometry technique.

Poster Presentation : **PHYS.P-212**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Excitation Wavelength Selective Control of the Reactivity of Photoacids

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Proton transfer has been widely investigated because of its biological and chemical importance. Excited-state proton transfer (ESPT) may provide valuable information about dynamical aspects of proton transfer reaction via real-time observation. Photoacids, which have acidic proton in the excited state, are representative examples showing ESPT [1]. As the ESPT of photoacids is a bimolecular reaction, the rate of reaction is at best several picoseconds in general because of the diffusion rate. Recently, a strong photoacid named as QCy9 is reported to have an ultrafast ESPT [2]. Furthermore, it has two absorption bands which show different photophysical properties. We have investigated the origin of two different absorption bands via various time-resolved fluorescence (TF) techniques.

The absorption spectrum with respect to the pH value shows that it is already weak acid in the ground state, with pKa≈4.3. In pH 1, with acidic form, there are two absorption bands in 400 nm and in 340 nm. Two different bands have same basic form fluorescence band but different acidic form fluorescence bands. When we excite the molecule with 400 nm, the ESPT rate is 100 fs. When the excitation wavelength is converted to 320 nm, the reaction is slower and shows a long lifetime even in the acidic band of fluorescence. The origin of two different proton transfer kinetics is the structural difference in the ground state. Using the DFT calculation, we found four different conformations in the ground state with similar energy. In conclusion, we found the photoacid which shows different reactivity with respect to the excitation wavelength.

[1] N. Agmon, J. Phys. Chem. A 109, 13 (2005).
[2] R. Simkovitch, N. Karton-Lifshin et al., J. Phys. Chem. A 117, 3405 (2013).

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Immobilization of lipid vesicle using His-tagged biocytin on a supported lipid bilayer.

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We developed a new scheme for surface attachment of lipid vesicle using His-tagged biocytin (His-biocytin) which is relatively easy to synthesize compared to the His-tagged lipid for single molecule study. We labeled supported lipid bilayers on a glass coverslip with His-biocytin and allowed nitrilotriacetic acid (NTA) containing lipid vesicle to bind to the membrane in the presence of Ni^{2+}. We employed a confocal fluorescence microscope to observe the specific binding of NTA-lipid containing lipid vesicle on the His-biocytin labeled membrane. Unlike conventional vesicle attachment scheme using a streptavidin-biotin binding, this method uses a reversible metal-chelate binding to create a new surface. To apply this method to single molecule study, we measured fluorescence lifetimes of TMR biocytin-streptavidin complex in the lipid vesicle. We found that the protein-dye complex in the lipid vesicle rotates freely and does not adhered to the inner surface of the lipid vesicle based on the fluorescence lifetime of the TMR biocytin bound to streptavidin in the lipid vesicle.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Gap-dependent diffusion kinetics for molecular hole dopants through MX_2-substrate

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Understanding molecular behavior in nanometer-scale confinement is important in various scientific fields and technological applications of low-dimensional material systems. In particular, interfacial molecular diffusion is known to be a key step of ambient charge transfer (CT) doping in two-dimensional materials supported on substrates. Its detailed mechanism and kinetics, however, have yet to be revealed. In this work, we investigated the space-resolved kinetics of CT in single-layer (1L) transition metal dichalcogenides (TMDs) of MX_2 (M = Mo, W and X = S, Se) using a redox reaction model where O_2/H_2O couples serve as a hole dopant.[1] As a charge density probe, photoluminescence (PL) spectroscopy and imaging were applied to four different TMDs supported on SiO_2 in a gas-controlled optical cell. For all TMDs, oxygen gas induced hole carriers, which could be reversed in Ar atmosphere. Interfacial diffusion of the molecular dopants was confirmed by spatial propagation of change in PL intensity from edges towards centers of samples. We also found that the diffusion was accelerated for samples with larger interfacial gaps between TMDs and supporting substrates. TMDs supported on sapphire and mica substrates will also be discussed in regard with possible roles of confined water layers in the CT reactions.[1] V. Chakrapani, J. C. Angus, A. B. Anderson, S. D. Wolter, B. R. Stoner, G. U. Sumanasekera, Science 318, 1424 (2007)

Poster Presentation : **PHYS.P-215**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Observation of non-Condon effects on intensity modulations of transient absorption signals

Jungsoo Ahn, Taiha Joo*

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Effect of non-Condon effect on transient absorption signals of indocyanine green molecule has been obtained using femtosecond transient absorption spectroscopy. Practicability of observation is, nevertheless, widespread; it is unfeasible to pinpoint the origin of observed oscillation in transient absorption or time-resolved fluorescence. When the oscillation are analyzed, it has been customary to apply the Condon approximation, that is, transition dipole moment change induced by molecular vibrational motion has been neglected. Consequently, a method of elucidation on the origin of observed intensity modulations deserves consideration. The method would be actualize through measuring the initial phase difference of the oscillations observed at the blue and red side wavelength of spectral band.

Poster Presentation : **PHYS.P-216**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Formation and Phase Behaviors of Binary Self-Assembled Monolayers on Au(111) by Coadsorption of Two Thiols with Geometrically Controlled Backbones

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Department of Chemistry, Hanyang University, Korea

Two-component mixed self-assembled monolayers (SAMs) are especially promising due to their strong potential to tune the physical and chemical properties of surfaces by changing the tail group, length, and chemical structure of the thiol molecular backbone. Therefore, SAMs have been utilized for various practical applications including pH-sensitive supramolecular switches, protein adsorption, organic field-effect transistors, and molecular electronic devices. Mixed SAMs on gold can be readily prepared using three methods: coadsorption of two different thiols, adsorption of asymmetric disulfides, and sequential adsorption. In this study, we investigated the surface morphology of mixed self-assembled monolayers (SAMs) formed by coadsorption of adamantanethiol (ADT) with a spherical cage backbone and other thiols with a different backbone (ethyl, decyl, and phenyl group) in 1:1 molar ratio ethanolic solution using scanning tunneling microscopy (STM) and cyclic voltammetry (CV). We found that phase-separated domains were prominently observed in SAMs formed by coadsorption of ADT and decanethiol, whereas homogeneous surface morphology was formed in SAMs by coadsorption of ADT and ethanethiol, suggesting that the surface structure of SAMs can be easily tuned by changing alkyl chain length of alkanethiols. In addition, structural changes of nano-interface according to the immersion time of each mixed thiol will be discussed in this presentation.

Poster Presentation : **PHYS.P-217**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Raman-pump power dependent artifact signal of trans-stilbene

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Femtosecond stimulated Raman spectroscopy (FSRS) is able to monitor the transient vibration modes of molecules within sub-picosecond time scale after photoexcitation. Especially, trans-stilbene and its derivatives which have trans-cis photoisomerization reaction have been variously studied because of large extinction coefficient and Raman activity. We have built above optical setup with a feasible resonant condition (S_n - S_1 state) and we performed Raman-pump power dependent experiment of trans-stilbene derivatives with a narrow spectral-resolution (sub-10 cm^{-1}) and a short time-resolution (80 fs). Though the first decay component assigned to intramolecular vibrational redistribution is reported by some groups, we revealed that it is the inevitable artifact of population depletion with high Raman-pump power. To support this results, we also had a non-resonant Raman experiment with Etalon that have a exponential pulse with a cavity lifetime in the time-domain. Therefore, I will present the optimized process for obtaining power-sensitive FSRS signal in resonance condition.

Poster Presentation : **PHYS.P-218**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Controllable Gold Nanoparticles Ablated by Pulse Laser in Organic Solvent for SERS Substrate

Hyeyeon Lee, Seung Heon Lee, Seung Jun Lee, Juhyeon Park, Tae Ho Kim, Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

Surface Enhanced Raman Spectroscopy (SERS) has currently investigated to analyze microscopic signals in sensors such as biosensing. Among many attempts to enhance the SERS effect, experiments to create hotspots of metal particles have been reported in various ways. In this study, we have synthesized Au nanoparticles (NPs) which have thin carbon layers with constant thickness by using ns-laser and investigated SERS effect. Controllable Au NPs are generated by ablating Au plate in water, acetonitrile and mixture in order to control carbon layers and remove amorphous carbon. We have investigated size and shape of Au NPs controlled in two solvents with transmission electron microscopy (TEM), UV-vis spectroscopy, micro-raman. By mixing two different solvents, the number of carbon layers on Au NPs are decreased, and it is found that the gaps of < 1 nm created by the carbon shell led to a strong plasmon effect. Since gaps which induce hotspot are formed, enhanced SERS signals from Au NPs treated by pulse laser are obtained by using Rhodamine 6G (R6G) as a target material.

Poster Presentation : **PHYS.P-219**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Crystal Structures and Photoluminescent Properties of Dimethyl Sulfonium Salts based on π-Electron Deficient Spacers

Juhyeon Park, Tae Ho Kim, Cheol Joo Moon, Sang Hun Yeon, Myong Yong Choi*, Jineun Kim*

Department of Chemistry, Gyeongsang National University, Korea

2,7-bis[3-(methylthio)propyl]-benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone (**1**)/ 2,6-bis[3-(methylthio)propyl]-benzo[1,2-c:4,5-c']dipyrrole-1,3,5,7(2H,6H)-tetrone (**2**) were synthesized by the reaction of 1,4,5,8-naphthalenetetracarboxylic dianhydride/benzene-1,2,4,5-tetracarboxylic dianhydride with 3-(methylthio)propylamine. Bis-dimethylsulfonium iodides **3** and **4** were prepared by methylation of **1** and **2** with iodomethane. Two compounds **3** and **4** were composed of central naphthalene diimide/pyromellitic diimide, terminal dimethylpropylenyl sulfonium groups ($Me_2SCH_2CH_2CH_2$-) and iodides, respectively. Crystal structures of **3** and **4** were determined by single crystal X-ray diffraction. **3** and **4** were crystallized in monoclinic $P2_1/c$ and $P2_1/n$ space group, respectively. **3** and **4** lie on the crystallographic inversion center. Bis-dimethylsulfonium iodide **3** is non-emissive, while **4** is emissive. The emission spectra of **4** showed maximum peaks at about 405nm and 576nm in the solution and solid state at room temperature, respectively.

Poster Presentation : **PHYS.P-220**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Effect of Different Solvents on the Properties of Copper Nanoparticles Produced Via Pulsed Laser Ablation and its Enhanced Catalytic Activity

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Copper nanoparticles with a range of different surface morphologies were synthesized by pulsed laser ablation method using a copper plate as a target in liquid media (deionized water, methanol, ethanol, 1-propanol, butanol, ethylene glycol, hexane and acetonitrile). Moreover, powder X-ray diffraction (XRD) analysis revealed that the species differ not only in shape, but also in composition. When laser ablation of a solid copper plate was carried out in acetonitrile, a core-shell nanostructure of copper@graphitic carbon (Cu@GC) and copper (I) cyanide particles were formed. While spherical and rod-like structured particles of copper (I) and (II) oxide was obtained in deionized water and methanol, respectively. The catalytic activities of the synthesized copper nanoparticles were evaluated for the reduction of 4-nitrophenol to 4-aminophenol, and nitrobenzene to aniline, as a model reaction. Based on the obtained results and pseudo-first order kinetics, the synthesized nanoparticles of copper (II) oxide and copper encapsulated in graphitic carbon layers demonstrated an enhanced catalytic performance towards the reduction of 4-nitrophenol and nitrobenzene. The enhanced catalytic activities of this catalysts might be due the unique surface morphologies and positive synergistic effect between copper nanostructures and graphitic carbon layer. The present investigation was revealed that the pulsed laser ablation of copper plate in various liquid medium is a facile method for producing of copper and copper-based nanoparticles with unique surface structure, compositions and act as an excellent catalytic material.

Poster Presentation : **PHYS.P-221**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fluorescence Correlation Spectroscopy of Gold Nanoclusters

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Nanoclusters are miniaturized nanoparticles of 1-3 nm smaller than nanoparticles and are homogeneous. Hydrodynamic radius of the nanoclusters in solution is important because the fluorescence properties are related to the size of the clusters such as aggregation-induced emission (AIE). Fluorescence correlation spectroscopy (FCS) employs photon correlation analysis of fluctuations in fluorescence intensity to gain insight into the diffusion of the samples such as hydrodynamic radius and average concentration. However, the fluorescence of AuNC is so weak that it is very difficult to obtain fluorescence correlation directly from AuNC. In this research, we synthesized thiolated gold nanoclusters (AuNC) and labeled the gold nanoclusters ($Au_{10\sim12}(SR)_{10\sim12}$, $Au_{15}(SR)_{13}$, $Au_{18}(SR)_{14}$, $Au_{25}(SR)_{18}$) with biotinylated fluorescent dye to measure fluorescence correlation and obtained the characteristic diffusion times AuNCs. We found that the diameters of dye labeled-Au NCs are ~2 nm based on the diffusion times obtained from FCS fits.

Poster Presentation : **PHYS.P-222**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Electronic and Vibrational Spectroscopic Studies of Jet-cooled 2-cyanoindole and Its water cluster, 2CI-(H2O)n (n = 0 - 3)

Hak Seung Ryu, Cheol Joo Moon[1], Myong Yong Choi[1,*]

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

In this study, 2-cyanoindole (2CI) has found some spectroscopic interest about excited in the gas phase. The excitation spectra of 2-cyanoindole (2CI) and its water clusters, 2CI-(H H_2O) H_n(n=1~3), have been measured by using mass-selected resonant two-photon ionization (R2PI) in the gas phase. For monomer, R2PI spectrum was obtained, but with abroad spectral feature. However, it was possible to observe sharp spectral peaks for 2CI-(H H_2O) H_{1-3} clusters upon adding water. Moreover, the origin band of each cluster shifted to the red frequency as the number of water increased. These result suggest that the addition of water molecules sufficiently lengthens the excited-state lifetime that we obtain a fully vibrationally resolved electronic spectrum. The transition energy of the origin band of the R2PI spectrum was compared with that obtained by density functional theory (DFT) calculations. Then, we obtained UV-UV hole-burning (UV-UV HB) spectra to identify the number of conformers in the 2-cyanoindole and their water clusters. Here report the structural information of 2CI water clusters by comparing the each IR-dip spectra and those from the theory. Further investigation on the structures of 2CI and its water clusters will be investigated and discussed by IR-dip spectroscopic studies in this poster. The spectroscopic properties of excited states in gas phase are investigated and discussed by comparing with those obtained from the theoretical calculations.

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Poster Presentation : **PHYS.P-223**
Physical Chemistry
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Novel plasmonic ZnO/Au/g-C_3N_4 nanocomposites for visible-light-active photocatalysts

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Novel ZnO/Au/graphitic carbon nitride (g-C3N4) nanocomposites were fabricated through a facile and eco-friendly three-step pulsed laser ablation method in liquid followed by calcination, without the use of a capping agent or surfactant. The as-prepared photocatalysts were examined by electron microscopic and spectroscopic techniques, and the results further confirmed the good dispersion of Au nanoparticles (NPs) on the surface of spherical ZnO particles and g-C3N4 nanosheets. The ZnO/Au/g-C3N4 nanocomposite exhibits substantially enhanced catalytic activity toward the degradation of methylene blue (MB) under visible-light irradiation. This improved photocatalytic activity of ZnO/Au15/g-C3N4 is attributed to the surface plasmon resonance of Au NPs and the synergistic effect between ZnO and g-C3N4. The boundary between ZnO/Au and g-C3N4 enables the direct migration of photogenerated electrons from g-C3N4 to ZnO/Au, which can easily retard the recombination of electron–hole pairs and boost the carrier separation efficiency. A reasonable MB degradation mechanism over the ZnO/Au/g-C3N4 photocatalyst is proposed on the basis of the results.

Poster Presentation : **PHYS.P-224**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of ZnO/Au/RGO nanocomposites using PLAL for Photocatalytic degradation of Organic pollutants.

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Herein, visible light active ZnO/Au/RGO ternary nanocomposites were successfully synthesized by Pulsed Laser Ablation (PLA) technique in liquid medium. The photocatalytic activity of as synthesized ternary nanocomposites was evaluated for the degradation of Methylene Blue and Rhodamine-B under visible light irradiation. The synthesized materials were characterized by UV-visible spectrometry, photoluminescence (PL), scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD). The optimal ZnO/Au/RGO showed the higher degradation efficiency than bare ZnO. The density of the Au nanoparticle and RGO nano matrix on ZnO could be altered by changing the concentration of gold and RGO as (5%wt, 10%wt, 15%wt) using laser irradiation and photo-deposition technique. This enhanced photocatalytic activity is attributed to the efficient separation and transfer of photo induced electron-hole pairs in ZnO/Au/RGO ternary nanocomposites. The superior photocatalytic activity revealed that the ZnO/Au/RGO ternary nanocomposites could be a promising material for waste water treatment and other environmental remediation applications.

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Electronic circular Dichroism Spectrar of L-Protonated Phenylalanine Ion Obtained Using Cold Ion spectroscopy

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chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Iltae Yoo, Han Jun Eun, Chang Wook Jeon and Nam Joon Kim*Department of Chemistry, Chungbuk National University, Cheoungju, KoreaCircular dichroism spectroscopy (CD) of jet-cooled chiral molecules provides conformation -specific CD spectra. Here, we have developed an efficient CD spectroscopic technique that can be applied to molecular ions produced by electrospray ionization and stored in a quadrupole ion trap. Using this CD spectroscopic technique, we obtained the first electronic CD spectra of L-protonated phenulalanine(L-H+Phe) ions using cols ion spectroscopy. The ECD spectra of L-H+Phe and D-H+Phe exibit well-resolved CD bands, which are mirror images to each orher. The sign of the vicronic bands in the spectra agree well with those simulated electronic CD spectra using the time-dependent density functional theory(TDDFT).

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

NiFe OER catalytic reaction study using in situ Sum-frequency generation spectroscopy

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

Water oxidation is an essential reaction for energy storage such as forming of hydrogen or hydrocarbons without accumulation of by-product. Unfortunately, This reaction is consist of a complex multistep, which adds a considerably large overpotential to the actual process. Although many studies have been conducted on OER catalysts with low overpotential and high stability, the specific catalytic reaction mechanism has not yet been elucidated. Among them, NiFe catalysts, which form layered double hydroxide (LDH) structures by potential, show excellent performance in alkaline conditions. The performance of the catalyst varies depending on the distance between the layers and the ratio of Ni and Fe. To understand this catalytic tendency and mechanism, it is important to use surface/interface selective spectroscopic method. Here, using vibrational sum-frequency generation (VSFG) spectroscopy, we selectively identified graphene electrode-electrolyte interfacial molecules. And we designed spectro-electrochemical (SEC) cell for in situ SFG experiment. In this work, using nonlinear spectroscopic method, we can observe that the hydrogen bonding network of the interfacial water molecules changes at each potential.

Poster Presentation : **PHYS.P-227**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

NiO as Back Ohmic Contact Hole Transport Layer to p-type doped CuBi2O4 for Photoelectrochemical Water Splitting

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Electrochemical synthesis methods were developed to produce $CuBi_2O_4$ (CBO), a promising p-type oxide for use in solar water splitting, as high surface area electrodes due to its optimal optical band gap and positive photocurrent onset potential. However, despite these favorable attributes, CBO photocathodes have shown limitations in charge carrier transport within CBO and across the interface with n-type fluorine doped tin oxide (FTO). To overcome this both limitations, a very thin NiO layer inserted between the FTO and CBO, since the importance of NiO is recently described as one of the capable hole transfer layers (HTL) for its hole transport property, stable electrode, easy process to form thinfilm and helps to full coverage deposition of CBO. In addition to that, Ag-doped CBO electrodes were also prepared by adding a trace amount of Ag^+ in the plating medium and co-depositing Ag with the Cu/Bi films. In the Ag-doped CBO, Ag^+ ions substitutionally replaced Bi^{3+} ions and increased the hole concentration in CBO. The utilization of NiO as an ohmic back contact to hole concentration increased Ag-CBO material achieved a positive onset potential of 1.16 V vs RHE and observed twofold improvement in current density. And, the photostability recover experiments were compared and studied with addition of protecting layer on surface. Prepared photoelectrodes optical and structural properties were examined well. This study offers new thoughtful for building progressed CBO photocathodes by thoroughly investigating photocorrosion as well as photoelectrochemical performance of high-quality CBO and Ag-doped CBO (ACBO) photoelectrodes for water splitting reactions.

Poster Presentation : **PHYS.P-228**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Effect of Tethering Probes on the Rotational Dynamics of a Polymer near the Glass Transition

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The segmental dynamics of polymer, which is the relevant dynamics of the glass transition, can be probed by analyzing the rotation of the fluorescent molecules in polymer matrices via imaging rotational fluorescence correlation microscopy. Although tethered probes have broad applicability, only the rotational dynamics of untethered probes has been studied. Therefore, we tethered probes to polymer by changing the length of the flexible linkers and the number of tethering points. The rotational dynamics of tethered probes was found to be slower than freely rotating probes due to the restricted motion by linkers, but the temperature dependence of polymer dynamics and the shape of the correlation decay were not changed. In case of the bigger size of untethered probe, rotational dynamics was slower than smaller probes as tethered probes, but its mechanism is different : probe averaged over different regions of the dynamics heterogeneity. As a result, if the size of the probes was corresponding to that of the dynamics heterogeneity of the host system, tethered probes exactly report dynamics related to glass transition, regardless of tethering conditions.

Poster Presentation : **PHYS.P-229**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

X-ray Absorption Study of Photo-Induced Tautomeric Interconversion of Co-dioxolene complexes

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Department of Chemistry, Yonsei University, Korea
[1]*Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Japan, Japan*

The metal-dioxolene complex, showing redox isomerization have been actively investigated due to their potential application possibilities in the magnetic switch. In this work, we have performed picosecond time-resolved X-ray absorption spectroscopy (XAS) studies on the cobalt K-edge of two different Co-dioxolene complexes (Co(Cat-N-BQ)(Cat-N-SQ) and Co(tpy)(Cat-N-SQ)PF_6, where Cat-N-BQ = 2-(2-hydroxy-3,5-ditert-butylphenyl-imino)-4,6-ditert-butylcyclohexa-3,5-dienone, Cat-N-SQ is the dianionic radical analogue, and tpy = 2,2′-6-2″- terpyridine) in toluene solution. 100 fs, 500 nm pump pulses initiate one-electron charge transfer from the radical semiquinonate ligand to the Co-metal center in the low-spin complexes. The subsequent electronic and geometrical changes associated with the formation of high-spin state of Co- dioxolene complexes are probed by 70 ps, 7.7 keV tunable X-ray pulses from Photon Factory Advanced Ring (PF-AR). Theoretical modeling of transient XAS spectra reveals that the bond-distances between Co and nearby ligand-atoms are lengthened in the high-spin state. These structural changes cause the spectral changes, which reflect altered hybridization of metal-3d, metal-4p, and ligand-2p orbitals accompanied by one-electron transfer process.

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Poster Presentation : **PHYS.P-230**
Physical Chemistry
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Tip-enhanced Raman spectroscopy of thiol monolayers on gold nanoparticle

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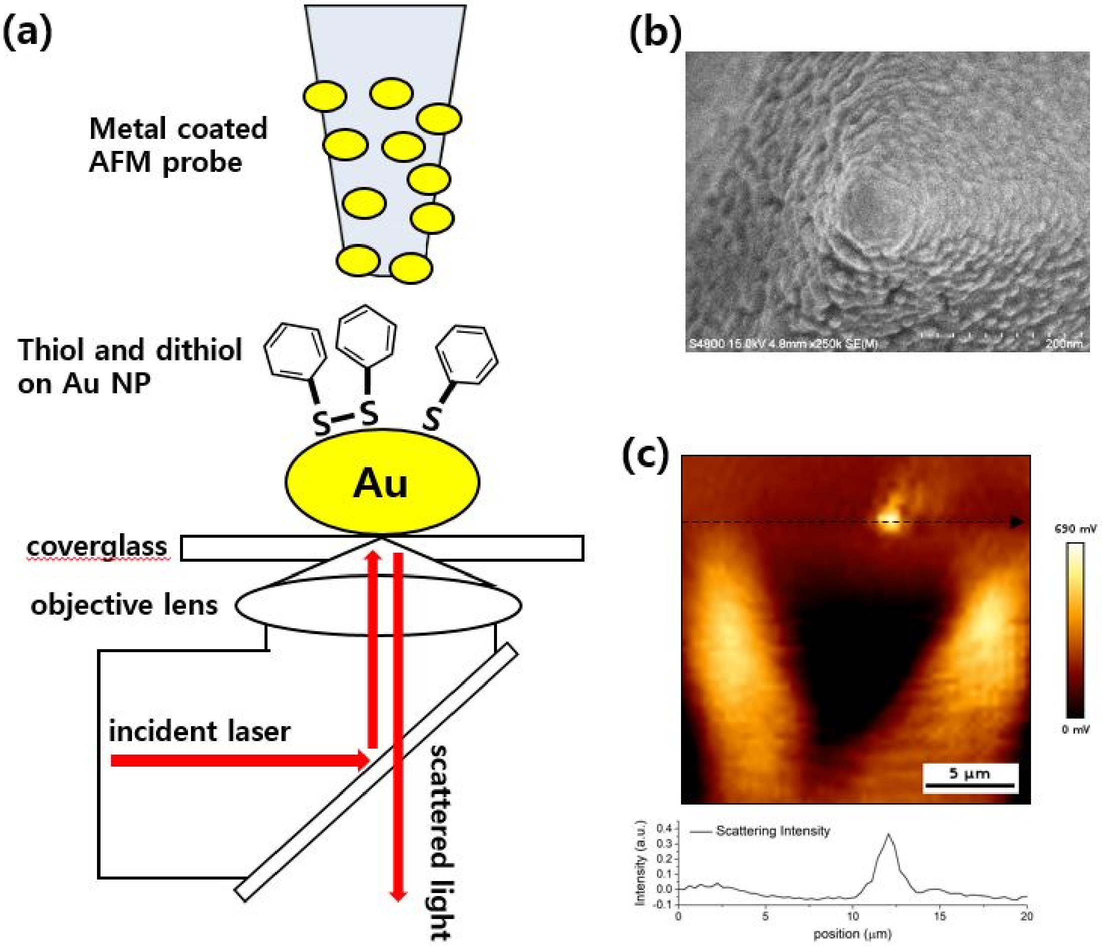
Functionalization of molecules on gold surface through thiol bonding provides fundamental building blocks for many fascinating complex nanostructures. Since self-assembled thiol monolayer plays key role in determining the yield and the quality of the complex nanostructures, chemical component analysis of gold surface in non-destructive way is highly desirable. In this presentation, we demonstrate tip-enhanced Raman spectroscopy on benzenethiol monolayer functionalized on gold nanoparticles. By positioning the atomic force microscopy probe coated with gold and silver respectively, in the close proximity of gold nanoparticles, Raman spectrum corresponding to benzenethiol is successfully acquired. Furthermore, we have observed clear differences in probe contamination trends depending on the coated metal species of the probe. Undesired bonding of analyte thiols to the surface of approached probes were more severe for gold coated probes comparing to silver coated ones. Our work demonstrates the surface characterization technique of gold nanoparticle based on tip-enhanced Raman spectroscopy with molecular monolayer sensitivity.


(a)
Metal coated AFM probe
Thiol and dithiol on Au NP
S
S
S
Au
coverglass
objective lens
incident laser
scattered light
(b)
S4800 15.0kV 4.8mm x250k SE(M)
200nm
(c)
690 mV
0 mV
5 µm
Scattering Intensity
Intensity (a.u.)
0.4
0.3
0.2
0.1
0.0
-0.1
0
5
10
15
20
position (µm)

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Poster Presentation : **PHYS.P-231**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Estimation of a molecule's excited-state absorption spectra by vibronic transition calculations

Joonyoung F. Joung, **Sungnam Park***

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Excited-state absorption (ESA) spectra are important for understanding the light-driven molecular processes observed in the transient absorption and steady-state photoinduced absorption experiments. Theoretical calculations of ESA spectra of a molecule have been quite challenging. Several theoretical advancements in the computation of ESA spectra have been made but currently available computational methods are limited for practical use and computationally expensive. In this study, we demonstrated a practical method to calculate the ESA spectra of a molecule by using vibronic transition calculations. Our method is shown to be reliable and computationally inexpensive and can be applicable to many molecular systems.

Poster Presentation : **PHYS.P-232**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Chemical application of machine learning to predict optical properties

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Machine learning has been applied to predict the physical and chemical properties of a molecule. In this work, more than 6000 combinations of chromophores and solvents and their various optical properties are collected to build the database. Based on the database, the machine learning is used to predict the optical properties, such as absorption and emission wavelength, fluorescence lifetime, quantum yield, and extinction coefficient. The results of our machine learning will be presented.

Poster Presentation : **PHYS.P-233**

Physical Chemistry

Exhibition Hall 1, THU 11:00~12:30

Molecular dynamics simulation study on ion-pairing dynamics in polar solvents

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In solutions, ions exist in different ionic forms: contact ion pair (CIP), solvent-shared ion pair (SIP), solvent separated ion pair (2SIP), and free ions. At a given temperature, the equilibrium among them is determined by inter-ionic interaction and ion-solvent interaction. In this study, we utilized molecular dynamics (MD) simulations to study the equilibrium of ion pairing between alkali metal ion and thiocyanate (SCN^-) in polar solvents. The effect of ion-ion interaction and polar solvent on the ion pairing equilibrium will be presented.

Poster Presentation : **PHYS.P-234**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Construction of 1-D ternary nanohybrid CdS/ZnS/Pt for high selective CO_2 reduction with water

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

Carbon dioxide the major contributor to climate change becoming increasingly apparent and worrisome due to its role as greenhouse gas. Conversion of anthropogenic carbon dioxide (CO_2) to value-added chemicals through solar driven catalysis considered as an appealing approach to tackle CO_2 emission challenges. Although materials developed to produce high energy fuels from CO_2 reduction with water, it is still a challenge to develop suitable, highly efficient and stable nanostructures for long time operation. Further, as CO_2 reduction reaction requires participation of multiple electrons, only nanohybrids involving two are more selective co-catalysts is beneficial. Herein, we report photo deposited Pt on core shell structured CdS-ZnS nanohybrid as durable catalyst for CO_2 reduction. The unique design integrates covering of CdS nanorods with ZnS shells and further photo reduction of H_2PtCl_6 onto CdS/ZnS in water-alcohol system. This delicate design accelerates the separation and transfer of photo generated charges, enhanced the photo absorption, reduced photo corrosion of CdS and facilitates abundant catalytic active sites. The as-synthesized CdS/ZnS/Pt nano hybrids are investigated for photocatalytic CO_2 reduction with water to produce CO and CH_4 in presence of Tri ethanol amine (TEOA) as hole (h+) scavenger. The optimized Pt-CdS-ZnS photocatalyst exhibited good stability for more than 42 hrs with unbroken rate of reaction for CO generation. The hybrid material realizes efficient solar-to-chemical energy conversion in suspension, demonstrating the potential of delicate structured materials are highly efficient and stable catalysts for CO_2 reduction into carbon feedstock fuels.

Poster Presentation : **PHYS.P-235**
Physical Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fluorescence calculation of exciplex state of magnetic field effect (MFE) peptoid using density functional theory

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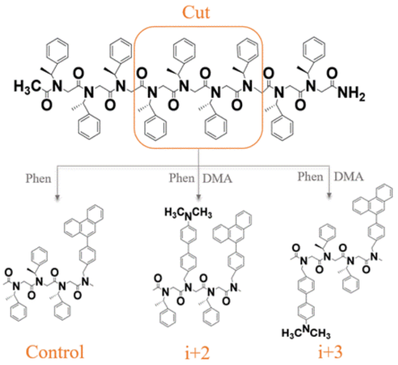
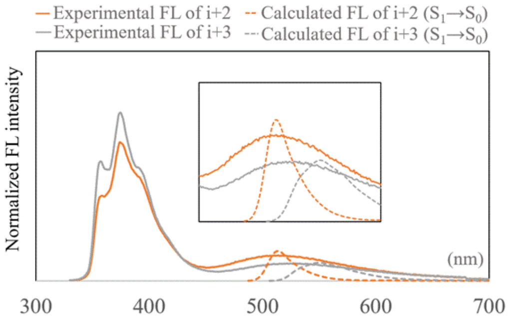
To understand the photophysical properties for the experimental fluorescence (FL) spectrum of magnetic field effect (MFE) peptoid structure with phenanthrene (Phen) and dimethylaniline (DMA), we investigated the vibrationally resolved FL spectrum of that obtained using time-dependent density functional theory (TD-DFT) and Franck-Condon and Herzberg-Teller (FCHT) calculation which were carried out using B3LYP-D3BJ/6-31G(d,p) level of theory. MFE peptoid structures were named the control, i+2, and i+3 according to the location of Phen and DMA. We found that the first excited state (S1) structures of i+2 and i+3 are the exciplex state which is an excited transient complex composed of electron-donor Phen and electron-acceptor DMA, which generated the new green FL spectrum at 500~600nm by charge transfer between Phen and DMA. Whereas, the calculated the FL spectrum of control with Phen only showed locally excited emission at 350~450nm by Phen. Therefore, MFE peptoid structure with exciplex state can produce a new emission band in a longer wavelength region than that of the locally-excited emission.


Cut
H$_3$C
NH$_2$
Phen
Phen DMA
Phen DMA
H$_3$C$_\text{N}$CH$_3$
Control
i+2
i+3


Experimental FL of i+2
Experimental FL of i+3
Calculated FL of i+2 ($S_1 \rightarrow S_0$)
Calculated FL of i+3 ($S_1 \rightarrow S_0$)
Normalized FL intensity
(nm)
300
400
500
600
700

Poster Presentation : **ANAL.P-77**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

One-pot synthesis of iron hydroxide hierarchical supraparticles

Hui Wu, Jaebeom Lee[1,*]

Department of Cogno-mechatronics Engineering, Pusan National University, China
[1]*Chemistry, Chungnam National University, Korea*

Iron hydroxide nanomaterials are extensively explored in catalysis, sensors, environmental protection, energy storage and biomedical applications. In this work, two different hierarchical iron hydroxide supraparticles with mesoporous structures were obtained by a facile, efficient and environmentfriendly method via a sodium sulfate-assisted one-pot reaction. Particularly, no templates or toxic materials are involved. By controlling the ratio of iron ions and sodium sulfate, the structure of the iron hydroxide supraparticles can be smartly tailored from hierarchical porous one-dimensional hemp rope-like structure to three- dimensional iron hydroxide supraparticles. A plausible formation mechanism has been proposed based on systematic investigation of the assembly process.

Poster Presentation : **ANAL.P-78**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Radiochemical Purification for ^{55}Fe Measurement

Kyungwon Suh

Radioactive Waste Chemical Analysis Center, Korea Atomic Energy Research Institute, Korea

The mission of Radioactive Waste Chemical Analysis Center in KAERI is to determine the radionuclides inventory in radioactive wastes according to Nuclear Safety and Security Commission (NSSC) No. 2017-60, "Waste Acceptance Criteria for low and intermediate radioactive wastes": to identify the radionuclides that make up more than 95% of the total radioactivity contained in the radoactive waste and specify that the concentration should be identified for the following:^{3}H, ^{14}C, ^{129}I, ^{99}Tc, ^{90}Sr, ^{55}Fe, ^{94}Nb, ^{59}Ni, ^{63}Ni, ^{58}Co, ^{60}Co, ^{137}Cs and ^{144}Ce. For the mission, chemical separation methods such as precipitation, ion-exchange chromatorgraphy, solvent extraction and extraction chromatography are necessary to determine the radioactivity of a difficult-to-measure radionuclides such as beta emitting nuculides because of the interference from co-existing radionuclides during the measurement.Herein, an optimally chemical separation condition for iron purification by the elimination of interference from co-existing radionuclides was demonstrated. In other words, ^{55}Fe should be individually separated before measurement by liquid scintillation counting due to the interference from calcium and nickel. Precipitation and solvent extraction or ion-exchange chromatography gave the selective iron separation from calcium and nickel. Precipitation by oxalate and phosphate showed a selective removal of calcium and nickel, respectively. MIBK extraction showed selective iron separation from each case. I will present this strategy for selective iron separation from calcium and nickel.

Poster Presentation : **ANAL.P-79**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

The case study of selective zirconium elimination for the determination of impurity elements in nuclear-grade zirconium alloys

Kyungwon Suh

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Zirconium is one of important elements in nuclear materials because of its excellent corrosion resistance in high temperature and pressure, sufficient mechanical properties and low neutron absorption coefficient. For nuclear applications, boron and cadmium in zirconium alloys should be less than 0.5 ppm because of their high neutron absorption cross-section. Therefore, it is necessary to quantify the amount of boron and cadmium in nuclear-grade zirconium alloys.Herein, the comparison between the conventional elimination method and selective precipitation by a heteropoly anion was presented: in the case of the conventional elimination method, tri-butyl phosphate extraction was applied, which did not give selective separation of boron and cadmium from zirconium. However, the precipitation by heteropoly anion showed selective elimination of zirconium meanwhile boron and cadmium were not precipitated. I will present these results in detail.

Poster Presentation : **ANAL.P-80**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Magnetic field-induced self-assembly of magnetoplasmonic nanoparticles into chain structures and chiroptical property

Ki-Jae Jeong, Dong-kyu Lee, Jaebeom Lee[1,*]

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[1]*Chemistry, Chungnam National University, Korea*

Helix is representative structures which shows optical activity. In nature, helical structures exist everywhere. From the molecular level for example biological molecules such as DNA, amino acid to cosmic phenomenon, planetary movement, gravitational wave, we can easily find the chiral and helical structures and vortex movements, and circularly polarized waves. The origin of chirality is coming from the structural asymmetry. Chiral structures such as helix have no any symmetric point, line, and plane. So it cannot be overlapped with its symmetric images. This figures can give different interactions with right- and left-handed circular polarized light. Here, we fabricated nature-inspired helix-mimetic optical activity modulator with self-assembled magnetoplasmonic nanochains. In the polymer gel and solution, we can assemble magnetic nanochain by external magnetic field. In addition, we can control its structures by physical force and magnetic field arrangement. As a results, circular dichroism signal intensities and sign can be changed.

Poster Presentation : **ANAL.P-81**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Voltammetric layer-by-layer biosensor for metabolite in human serum

<u>Yunpei Si</u>, Hye Jin Lee*

Department of Chemistry, Kyungpook National University, Korea

The metabolite level in human body is associated with the health condition and disease status. An electrochemical layer-by-layer (LbL) biosensing platform was demonstrated for highly sensitive and selective determination of metabolite by self-assembly of oppositely charged layers on screen printed carbon electrode (SPCE) surface. The developed sensing platform was applied in both normal human and myocardial infarction patient serum samples. The sensing results were further validated by a commercial detection kit and liquid chromatography-mass spectrometry (LC-MS) technique.

Poster Presentation : **ANAL.P-82**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Amperometric detection of neurotransmitter molecules using chemically modified screen-printed carbon electrodes

Jingjing Li, Hye Jin Lee*

Department of Chemistry, Kyungpook National University, Korea

Neurotransmitter species play critical roles in human physical and physiological functions involving blood pressure, mood and so forth. In this work, an amperometric biosensor was developed for the highly selective and sensitive detection of the neurotransmitter molecule using chemically modified screen-printed carbon electrodes. Cyclic and differential pulse voltammetry were used to investigate the electrochemical performance of the developed sensor. This neurotransmitter sensor will be applied to normal human and patient biological samples in the further.

124th General Meeting of the Korean Chemical Society
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Poster Presentation : **ANAL.P-83**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Alkaline Ionic Liquid Electrolytes

Muhammad Salman, Hye Jin Lee[1,*]

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

To meet the increasing demand for clean and sustainable energy, ionic liquids electrolytes are becoming alternate electrolytes in fuel cell due to less corrosive comparing to alkali metal based electrolytes like KOH. In this work, novel alkaline ionic liquid electrolytes were synthesized and their properties were studied. All the results indicate that the synthesized ionic liquids are promising in energy and environmental applications.

Poster Presentation : **ANAL.P-84**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Electrochemical Sensors for Alkaline Fuel

Dieudonne Tanue, Hye Jin Lee*

Department of Chemistry, Kyungpook National University, Korea

Fuel cell is an environmentally friendly energy generating source and there is increasing demand for the development of sensors for fuel cell application. Herein, we report an electrochemical sensor based on chemically modified gold electrode for monitoring fuel concentrations. The electrochemical characteristics and sensing performance of the fabricated sensor were investigated by a series of electrochemical techniques. The results indicate the potential application of the sensor in alkaline fuel cells.

Poster Presentation : **ANAL.P-85**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Near-Infrared Molecularly Imprinted Polymers-Based Sensor for Ultrasensitive Detection of Pharmaceutical Residues in wastewater

Mohamed ragab elsayed Ali, **Salah Mahmoud Tawfik Ahmed**, **Yong-Ill Lee***

Department of Chemistry, Changwon National University, Korea

One of the alternative techniques for determining pharmaceuticals and their metabolites in the aquatic environment is the use of molecularly imprinted polymers (MIPs) as recognition systems. MIPs are tailor-made artificial receptor sites in a polymer, which possess good affinity and selectivity. This work presents the design of new optical sensor-based MIP for the detection of Carbamazepine (CBZ) as one of the most frequently detected pharmaceutical residues in wastewater. MIP was prepared via *in situ* photopolymerization process using upconversion nanoparticles (UCNPs), CBZ, N-allyl-3,4,5-trihydroxybenzamide, (E)-N-acryloyl-3-(3,4-dihydroxyphenyl)acrylamide and 1-(carboxymethyl)-4-vinylpyridin-1-ium bromide, ethylene-glycol dimethacrylate, eosin Y/ triethylamine (TEA) as fluorescent materials, template, functional monomers, cross-linking agent, and an initiating system, respectively. Our method utilizes the internal visible light emitted from UCNPs upon photoexcitation with near-infrared radiation, to locally photopolymerize a thin polymer shell of the MIP around the UCNPs. The TEM images of this hybrid showed an ultrathin shell of 2.5 nm thickness. Under optimum conditions, the results of the fluorescence quenching analysis showed excellent sensitivity (LOD, 28.5 pM) with good linear ranges of 0.5 nM to 500 μM for CBZ and a correlation coefficient of 0.992. Moreover, the practical application of the developed sensor for CBZ detection in tap and river water samples has been successfully described with satisfactory recoveries of 98.24-104.23% and RSD less than 5%. This work offers a novel facile strategy to develop a fluorescent sensor with selective, rapid and accurate detection of CBZ in the wastewater.

Keywords: molecular imprinting polymer, *in situ* photopolymerization, UCNPs, CBZ.

Poster Presentation : **ANAL.P-86**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Colorimetric paper based probe for the Detection of Amine-Containing Gases

DaeHyun Kwon, Bui The Huy[1], Yong-Ill Lee[1,*]

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

In this study, we propose a highly accurate, selective, and low-cost probe based on a paper based substrate for the detection of ethanolamine ($NH_2CH_2CH_2OH$), dimethylamine ($(CH_3)_2NH$), and trimethylamine ($(CH_3)_3N$) in the gaseous state at parts per million scale. The probe was prepared from seven different dyes, which were deposited on the paper substrate. The color change of dyes on the probe by amine gases was analyzed using red, green, and blue (RGB) values extracted from the images obtained with a smartphone app. To distinguish three amine gases, the chemometric tools consist of Principal Component Analysis (PCA), and Hierarchical Cluster Analysis (HCA) methods were applied. The proposed probe was applied for real samples with high recoveries. Our developed probe has a potential to be able to provide an early warning of natural gas pollution **Keyword:** colorimetric, gas sensor, amine detection, paper based device

Poster Presentation : **ANAL.P-87**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Photocatalytic degradation of sulfadiazine based on visible light-responsive Fe-doped carbon nitride

Qi Ou, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Nowadays, antibiotics have become a new source of pollution, and the abuse of antibiotics is becoming more and more harmful to the environment and human health. Therefore, it is of great significance to use different treatment techniques to remove antibiotics from water. In this study, porous iron doped graphitic carbon nitride (Fe/g-C_3N_4) with outstanding photocatalytic ability is synthesized and used for the degradation of SDZ successfully. The microstructure and optical properties of the Fe/g-C_3N_4 were characterized by UV-vis DRS, FT-IR, SEM-EDS, XRD, XPS, ICP-OES, PL and EIS. The results show that iron is successfully doped into g-C_3N_4, and the doping of Fe^{3+} significantly improves the photocatalytic activity. Compared with undoped carbon nitride, Fe/g-C_3N_4 has a porous structure, a lower band gap, improved separation efficiency of photogenerated electron and holes, a wider light absorption range and enhanced light absorption. Under white LED light irradiation, and Fe/g-C_3N can almost completely degrade SDZ with a degradation efficiency as high as 99.5%, whereas only 55% for g-C_3N_4. The degradation of SDZ by Fe/ g-C_3N_4 has the advantages of simple operation, high degradation efficiency and easy practical application. Besides, Fe/g-C_3N_4 also can be used for the degradation of other antibiotic pollutants in water. This work provides insight into the rational design of carbon nitride modification and photocatalytic degradation of other organic pollutants, and is expected to be used in practical applications. **Keywords**: Fe^{3+}-doped graphitic carbon nitride; Sulfadiazine; Photocatalytic degradation

Poster Presentation : **ANAL.P-88**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Chemiluminescent probes-based paper strips for detection of influenza

Jinsol Han, Sharipov Mirkomil, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

According to the World Health organization (WHO), millions of people are infected by influenza virus each year. Traditional diagnosis methods require high cost equipment and technician for diagnosis of influenza virus. Last decade, the development of alternative diagnosis techniques for influenza has received a tremendous attention of scientist. The emerging paper-based analytical devices (µPAD) has shown their potential as low cost and easy to use method in detection of several toxic molecules. Moreover, the availability as renewable natural resources of natural cellulose fibers, low cost, recyclability, and the possibility to modify the surface of the paper with sensing molecules such as fluorescent probe or chemiluminescent is promising in development of novel, low-cost and easy to operate sensing material. Unlike fluorescent probes, the emerging chemiluminescent probe do not require light excitation, resulting in higher sensitivities and signal-to-noise ratios. In this work, we aim to develop chemiluminescent derivative-based µPAD that is selectively activated in the presence of influenza virus. µPAD was designed via stacked system to ensure to deliver the influenza virus to the target area after deposition onto µPAD.**Keywords:** chemiluminescent,µPAD,infulenza,detection

Poster Presentation : **ANAL.P-89**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

The determination of folic acid using paper-based analytical devices

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

Department of Chemistry, Changwon National University, Korea

Folic acid (FA), known as Vitamin B9, pteroylglutamic acid (PGA) or folate, is a water-soluble vitamin and has been confirmed as a significant nutrient in humans and animals. A paper-based analytical device (PADs) for the determination of folic acid (FA) was designed using rhodamine B derivative-Cu^{2+} complex as a color indicator. The structural change of rhodamine B derivatives to be the ring-open forms (pink color) was enhanced by adding folic acid. The mechanism is based on the improvement of electron transfer from rhodamine B derivatives to Cu^{2+} in the presence of folic acid. The variation in color intensity can be either tracked by a UV-vis spectrophotometer or a paper-based analytical device in which the color intensity variation was operated with Red, Green, and Blue components (RGB) analysis. The detection limit and linear relationships were measured. The method showed a reliable performance for determination of folic acid in the real samples. **Keywords:** derivative, vitamin, paper-based analytical device.

Poster Presentation : **ANAL.P-90**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Novel $ZnBi_2O_4$-graphite Composites as Highly Active Visible-Light Photocatalyst for the Mineralization of Rhodamine B

Truong Thi thuy, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Novel photocatalyst from composite of zinc bismuth oxide ($ZnBi_2O_4$) and graphite hybrid composites was prepared via a co-precipitation method. The photodegradation activity of prepared $ZnBi_2O_4$-graphite hybrid composites were tested on rhodamine B (RhB) solutions under visible-light irradiation. The prepared composite exhibited excellent photocatalytic activity, leading to more than 95% of RhB degradation at an initial concentration of 50 $mg.L^{-1}$ with 1.0 g catalyst per liter in 150 min. The excellent visible-light photocatalytic mineralization of $ZnBi_2O_4$-1.0graphite in comparison with pristine $ZnBi_2O_4$ may be attributed to synergetic effects, charge transfer between $ZnBi_2O_4$ and graphite, and the separation efficiency of the photogenerated electrons and holes. The results demonstrate the feasibility of $ZnBi_2O_4$-1.0graphite as a potential heterogeneous photocatalyst for environmental remediation.

Poster Presentation : **ANAL.P-91**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Mineralization of Indigo Carmine Using $ZnBi_2O_4$-Bi_2S_3 Composites under Visible light

TaeJun Ju, Dang Nguyen Nha Khanh, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Novel highly visible-light active $ZnBi_2O_4$-Bi_2S_3 photocatalysts have been synthesized by a simple two-step co-precipitation and hydrothermal method. The efficiency of the prepared $ZnBi_2O_4$-Bi_2S_3 composites was evaluated for the degradation of Indigo carmine in aqueous solutions under visible light irradiation. The photocatalytic activities of the prepared $ZnBi_2O_4$-Bi_2S_3 composites was higher than that of pristine $ZnBi_2O_4$. This enhancement could be attributed to synergetic effects, charge transfer between $ZnBi_2O_4$ and Bi_2S_3, as well as the separation efficiency of the photogenerated electrons and holes. These results demonstrate the feasibility of utilizing $ZnBi_2O_4$-Bi_2S_3 as potential heterogeneous photocatalysts for environmental remediation.

Poster Presentation : **ANAL.P-92**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Optical sensing of triclosan with Fluorescence of upconversion nanoparticles composed potassium permanganate

Seong-Soo Lee, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

Triclosan (TCS) have been widely used in a lot of manufacturers as a preservative and a chronically toxic compound that adversely affects biological organisms and human health. In this work, optical features of upconversion nanoparticles (UCNPs) were used to develop a simple and rapid method for detecting TCS. A novel optical sensor of TCS is designed based on carboxylic group functionalized $NaYF_4:Yb^{3+}/Er^{3+}$ UCNPs coated with potassium permanganate ($KMnO_4$). The TCS sensor is able to do the non-autofluorescence, sensitive, and selective sensing through the “turn off-on fluorescence” technique by fluorescence resonance energy transfer (FRET). The FRET between the $KMnO_4$ and UCNPs occurs under an Near-infrared excitation at 980 nm resulted “turn-off fluorescence”. The sensor becomes “turn-on fluorescence” with the presence of TCS because TCS reduces $KMnO_4$. Recovering the fluorescence of UCNPs has ability to detect TCS. The resulting sensor showed an excellent response to TCS with 0.2 μM of a limit of detection in optimized conditions. **Keywords:** Triclosan, UCNPs, FRET

Poster Presentation : **ANAL.P-93**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Novel Fluorescence “Turn off-on” sensors for Highly Sensitive Detection of Spermine Based on Amphiphilic Polythiophene Nanohybrids

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

Department of Chemistry, Changwon National University, Korea

New optical sensors based on CdTe quantum dots coated with amphiphilic polythiophenes , namely, P1QDs and P2QDs, were developed for the detection of heparin and spermine. The emission of the P1QDs and P2QDs is found to be quenched in the presence of heparin by electron transfer mechanism through electrostatic and hydrogen- bonding interactions. Upon the addition of spermine, heparin has been removed from the surface of P1QDs and P2QDs due to the strong electrostatic interactions between spermine and heparin, which showed remarkable fluorescence recovery of the sensors. Under optimum conditions, both P1QDs and P2QDs sensors displayed limits of detection as low as 1.59 nmol L^{-1} and 0.88 nmol L^{-1} with linear ranges of 1–11 μmol L^{-1} and 1–10 μmol L^{-1}, for heparin , respectively. P1QDs and P2QDs also showed limits of detection for spermine of 2.90 nmol L^{-1} and 1.66 nmol L^{-1} with linear ranges of 0.05–15 μmol L^{-1} and 1–12 μmol L^{-1}, respectively. Moreover, the sensors presented high selectivity to heparin and spermine over common interfering substances. Finally it is successfully applied to rapid detection of heparin and spermine in real serum samples.**Keywords**: amphiphilic polythiophene nanohybrids, heparin, spermine, fluorescence sensors, serum, electron transfer

Poster Presentation : **ANAL.P-94**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Anlalyzing and switching chiral structure with magnetoplasmonic nanoparticles.

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Department of Cogno-Mechatronics Engineering, Pusan National University, Korea
[1]*Chemistry, Chungnam National University, Korea*

Nanomachines are synthetic assemblies that switch between defined molecular conformations upon stimulation by external triggers. Previously, our group arranged different types of magnetoplasmonic nanoparticles into 1-3D metastructure by controlling ligands, solvent's surface tension and external magnetic field. It is well known that assembled nanoparticles made new localized surface plasmonic modes and this can be observed as light absorbance on specific wavelength and chirality of the assembled structure can be detected by circular dichroism. Recently researchers developed the concept of dynamic plasmonics which means the studies of plasmonics on nanostructure has changeable morphology. Snapshot image and spectra of moving structure is detected. The concept suggested in this presentation shows one type of 4D self-assembly which means controlling the dynamicity of the arrays of nanoparticles. Not only taking snapshots of moving nanostructures, movement of nanostructure can be remote controlled. Between two layers of 1D structured nanoarray with an angle, rotational mode of the particles between the layers can be reversibly controlled by tuning the wavenumber in that area. This work is considerable to use in tunable plasmonic devices, which can be used as nanomachines, chemical sensors and telecom applications.

Poster Presentation : **ANAL.P-95**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis, dispersion, tribological performance of alkyl functionalized graphene oxide as an oil lubricant additive and synergistic effect with WS_2

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

Department of Chemistry, Keimyung University, Korea

Graphene and WS_2 has been reported as an excellent lubricant additive for reducing adhesion and friction, when coated on the various surfaces as an atomically thin material with low surface energy. GO is various methods have been proposed to enhance the physical properties of GO by its reduction, because it is difficult to apply GO to hydrophobic lubricant due to the large numbers of oxygen functional groups and the remarkably poor physical properties. To solve this problem First, We have painted a long alkyl chain of graphene oxide (GO) to improve the dispersion of oil-based lubricants with greatly enhanced lipophilicity. Second, a gelator is used for dispersion to improve lubrication performance. Alkyl functionalized GO is synthesized by reacting NH2-GO with butyl chloride, hexyl chloride, octyl chloride, decyl chloride, dodecyl chloride, tetradecyl chloride in ethanol under reflux, then 0.1wt% of alkyl functionalized GO are added into the base oil (PAO oil) and oil which containing WS_2. and then, ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene is investigated by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), and Scanning electron microscope (SEM). The tribological tests are performed with a tribometer via ball-on-disk test mode.

Poster Presentation : **ANAL.P-96**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Characteristics and Electrochemical Performance of Graphene/Silicon/Carbon nanofibers Composite films as Anode Material for Binder-Free Lithium ion Secondary Batteries

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

Department of Chemistry, Keimyung University, Korea

We report the interfacial study of a Graphene/Silicon/Carbon nanofiber Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon nanofibers (CNFs) were grown via chemical vapor deposition method with an iron-copper catalysts. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 700℃, and maintained for 30 min to synthesize CNFs. GO aqueous dispersion was added into the Silicon/CNFs solution, and the mixture was sonicated for 2h to obtain a GO/Silicon/CNFs aqueous dispersion. Electrode was fabricated by flow-directed vacuum filtration of GO/Silicon/CNFs aqueous dispersion through a filter membrane (90 mm in diameter and 0.22 μm in pore diameter) followed by air drying and peeling off from the filter. Subsequently,the composited GO/Silicon/CNFs was heated up to 550℃ at a rate of 10℃ min-1 in a quartz tube furnace with an argon flow,and maintained for 2h to form a rGO/Si/CNFs composite film. The morphologies, compositions and crystal quality of the prepared rGO/Silicon/CNFs composites were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of rGO/Silicon/CNFs composites as an anode of Lithium ion secondary batteries were investigated using two-electrode coin-type cell. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester.

Poster Presentation : **ANAL.P-97**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Development of Novel Upconversion Nanoparticles Functionalized with Amphiphilic Conjugated Polymer for Alprenolol Detection

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

Department of Chemistry, Changwon National University, Korea

Upconversion nanoparticles (UCNPs) are photoluminescence (PL) materials in which lower-energy excitation is converted into higher-energy emission via multi-photon absorption processes. In this research, a novel amphiphilic conjugated polymer was synthesized to act as functionalizing agents for $NaLuGdF_4:Yb^{3+}/Er^{3+}$ UCNPs. The UCNPs coated with amphiphilic conjugated polymer were characterized by using FTIR, ^{1}HNMR, TGA, SEM, TEM, UV, and PL instruments. These materials were used as optical sensor to detect Alprenolol which is kind of high blood pressure treatment. Developed sensor displayed good analytical performance such as low limits of detection, and good linearity. Furthermore, the sensor was successfully applied to analysis the level of alprenolol in human urine and serum samples with good recoveries. **Keywords**: Upconversion nanoparticles, amphiphilic copolymer, optical sensor, alprenolol, biofluids.

Poster Presentation : **ANAL.P-98**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A novel microfluidic paper-based analytical device coupled with mass spectrometry for biomarker detection in biofluid

Shavkatjon Azizov, Sharipov Mirkomil, Jae-Min Lim, Sarvar Kakhkhorov, Salah Mahmoud Tawfik Ahmed, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

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

Poster Presentation : **ANAL.P-99**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

SYNTHESIS OF MIXED METAL OXIDES-REDUCED GRAPHENE OXIDE HYBRID CATALYSTS FOR PHOTODEGRADATION OF INDIGO CARMINE

Dang Nguyen Nha Khanh, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

A novel series of $ZnBi_2O_4$/rGO hybrid catalysts were synthesized via co-precipitation method. The as-prepared catalysts were characterized by X-ray diffraction, Fourier transform infrared, UV-vis diffuse reflectance spectra, Field-emission scanning electron microscopy and Transmission electron microscopy techniques. The photocatalytic activities of $ZnBi_2O_4$/rGO catalysts was conducted using Indigo Carmine, and the $ZnBi_2O_4$/rGO offered better degradation of pollutants as compared to pristine $ZnBi_2O_4$. Among them, $ZnBi_2O_4$/rGO (rGO = 2%) owned the best photocatalytic activity. The enhancement of photocatalytic properties of $ZnBi_2O_4$/rGO indicates that the existence of rGO improved moving of photoinduced electrons from $ZnBi_2O_4$ to rGO, which effectively separation of the photoinduced electron-hole pairs in $ZnBi_2O_4$. The $ZnBi_2O_4$/rGO can be considered as a promising photocatalyst for dye waste water treatment.

Keywords:$ZnBi_2O_4$/rGO hybrid catalysts, Indigo Carmine, visible-light irradiation, photodegradation

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ANAL.P-100**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Determination of heat of formation using bomb calorimetric analysis for energetic materials

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Agency for Defense Development, Korea

In the field of energetic materials, heat of formation(HOF) is one of the important properties. Because density and HOF are essential components for estimation of performance. There are two ways to determine HOF value. First onw is calculation using particular code. Second one is to get the value by heat of combistion(HOC) using bomb calorimetric analysis(BCA) experimentally. HOC could be easily converted to HOF by Hess's law.For BCA experiments, small amount of sample is needed. So it is possible to estimate performance properties in the lab scale. Even BCA method is well known for determination of HOF, values of energetic materials are quite variable.Here in, we described BCA experimental results and consideration to determine HOF of high energy materials.

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Poster Presentation : **ANAL.P-101**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Development of QSAR modeling of fat-air and brain-air partition coefficients

Ja won Shin, Hyung Sik Jo, Sung Kwang Lee*

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The volatile organic chemicals (VOCs) inhaled through the respiratory tract transfer into the tissues through the lungs and blood, causing biological and toxicological problems. The partition coefficients from air to fat or brain can be useful for toxicity studies, drug development, and risk assessment.In this study, we were tried to develop predictive QSAR model to predict the partition coefficient of chemicals from air into fat or brain. Diverse chemicals with fat or brain-air partition coefficient data measured in human and mice tissues were used to develop QSAR model. Several machine learning methods, such as multiple linear regression, support vector machine, and random forest method were used as the algorithm of model development. In addition, model development was performed by combining the validation methods and the feature selection methods. The developed QSAR model not only predicts the partition coefficients of the VOCs, but also serves as input for PBPK modeling to predict dose-response curves.

Poster Presentation : **ANAL.P-102**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

In silico approach for predicting blood-air partition coefficients by QSPR method

Chanhong Min, Hyung Sik Jo, Sung Kwang Lee*

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Physiologically based pharmacokinetic modeling (PBPK modeling) has recently been used in the process of drug discovery and predictive toxicology. In particular, one of the main parameters, especially in respiratory-related PBPK modeling, is the blood-air partition coefficient (PBA), which is a physicochemical property that can indicate the amount of chemical entering the body through the respiratory tract.In this study, diverse chemicals with the PBA measured in human and mice the experiment were used to construct predictive QSPR models. The algorithms used in the predictive QSPR model are multiple linear regression analysis (MLR), support vector machine (SVM), and random forest methods. The developed QSPR model is expected to help explain the mechanism of inhalation toxicity through the distribution of chemicals in organs by predicting the PBA of organic chemical. ※ AcknowledgementThis research was supported by a grant (18182MFDS466) from the Ministry of Food and Drug Safety in 2019.

Poster Presentation : **ANAL.P-103**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Identification multidisciplinary function and analysis active chemical compound structure of natural biological resources that were collected from Southern-east asian countries

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This study aims to derive multi-function material from biological natural resources and also to identify its chemical structure. Candidate materials were collected from southern-east asian countries and one-hundred samples were provided for the screening of functional materials. First, dried samples were homogenized and extracted with 70% ethanol and then antimicrobial activity was identified using conventional 'paper disc assay' against infectious pathogens including *S. pseudopneumoniae*, *S. aureus*, *E. coli*, *P. mirabilis*, and *C. albicans*. Antioxidant activity was also validated by conventional ABTS(2,2′-azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid)) assay and effect of cellular ROS concentration was characterized using 'DCF-DA'-based cell staining approach. After 1st screening of antimicrobial activity with paper disc assay, IC_{50} values of derived candidates were characterized for the quantification of antimicrobial activity using alamarBlue-based cell viability assay. Finally, one of the candidates was characterized which has both antimicrobial and antioxidant activities. The IC_{50} values of X were identified as 0.294, 2.340, 2.175 and 3.699 mg/ml against *S. pseudopneumoniae*, *S. aureus*, *P. mirabilis* and *C. albicans* respectively. Moreover, the IC_{50} value of antioxidant for X was calculated as 4.157 μg/ml. Then, active chemical compound was purified by fractionation using prep-HPLC. The activities of antimicrobial and antioxidant were confirmed with paper disc-based susceptibility test and ABTS assay respectively. Finally, their cellular action mechanism and biocompatibility were also identified.

Poster Presentation : **ANAL.P-104**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Electrochemical Detection of Lung-Cancer Specific Exosomal miroRNA

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Exosomes contain microRNAs that can be a marker for early detection of cancer. We developed an amperometric sensor to detect engineered miR-21(Eng-miR-21) from exosome. The working probe was fabricated through the immobilization of complementary sequence (CP) of engineered miR-21 in SPCE/gold nanoparticles (AuNPs)/conductive polymer layer and bioconjugates contain Hydrazine(Hyd), P53 protein attached to AuNPs. P53 protein selectively binds to double-stranded Eng-miR-21/CP DNA and Hyd nonenzymatically catalyze the reduction of $H2O2$ to generate an electrochemical signal. Working probe layers were characterized through cyclic voltammetry(CV), electrochemical impedance spectroscopy(EIS) and X-ray photoelectron spectroscopy(XPS). The proposed biosensor showed excellent analytical performances in terms of sensitivity, selectivity and specificity.

Poster Presentation : **ANAL.P-105**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Resonance Raman Analysis of Korean Traditional & Modern Pigment

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Raman spectroscopy is a non-destructive and effective spectroscopic tool when investigating chemical components of materials. It can establish the molecular composition, physical structure and chemical binding of pigments analytes by measuring inelastically scattered photons incorporating molecular vibrational information following laser incidence. Since this method does not cause direct damage to the sample, it has great advantages in analyzing samples with artistic works and cultural heritages. However, coloring samples, such as pigments, may have difficulty obtaining desired data due to strong fluorescence in Raman analysis. To reduce fluorescence interference and to increase Raman efficiency of Korean painting pigments, we applied multiple lasers of different wavelength and recorded Resonance Raman scattering (RSR). Obviously, the relative intensity of fluorescence and Raman scattering varies pigments depending on the electronic energy states of pigments. Thus, the selection of excitation wavelength is the most basic steps in the Raman analysis of art and archeology and the next step is to correlate the color and chemical structure with resonance Raman scattering efficiency. In this work, we investigated the electronic absorption/emission spectra and Raman spectra of various traditional and modern Korean paints. Resonance and non-resonance Raman spectra were obtained at 5 excitation wavelengths. Through these spectra, we analyzed the correlation between absorption, emission and Raman.

Poster Presentation : **ANAL.P-106**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Carbon-polymer composite electrode by 3D-printing for heavy metal ions detection

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A functionalized 3D printed carbon-polymer composite electrode (3D-CPE) was prepared by 3D printing technique, which is compatible to a 3D-CPE in anodic stripping analysis of heavy metal ions (HMIs: Zn(II), Cd(II), Pb(II), Cu(II), and Hg(II)). The preparation method and utilization of the 3D printed composite electrode in anodic stripping analysis are described. The sensor surface was characterized using electrochemical and surface analysis methods. Experimental variables that affect the response signal, such as pH, deposition time, and ratio of 3D-CPE were optimized. The 3D-CPE exhibited a dynamic range between 0.5 ppb and 1.0 ppm with the detection limit of 0.04 ppb. Application of this electrode technique is very promising for environmental or industrial field analysis because of its simplicity of treatments.

Poster Presentation : **ANAL.P-107**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of whitlockite nanocrystals in tri-solvent system and biocompatibility evaluation

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Whitlockite (WH, Ca18Mg2(HPO4)2(PO4)12) is the second most abundant biomineral in human bone and has attracted attention as a novel bone regenerative material. It has been proven to enhance growth and promote osteogenesis of stem cells. However, investigating the mechanism of crystal formation in pure phase WH nanocrystals remains a challenge. In this study, a novel synthesis method of WH nanocrystals is introduced using a tri-solvent system of solid-liquid-solution (SLS). Precursor’s ratio and reaction solvent composition were optimized to grow WH nanocrystals with tunable sizes, morphology, and different surface properties. Molecular dynamics (MD) simulations elucidated the growth mechanism of WH nanoplates (M1.5). Computational finite element method (FEM) simulations were carried out to reveal the solvent effect in the reaction. The biocompatibility of the crystals was evaluated in human osteosarcoma cell line (MG63) treated with 0.16 to 100 μg mL-1 of M0, M1.5, and P10 up to 7 days. The cell proliferation and alkaline phosphatase (ALP) activity assay of human bone marrow derived mesenchymal stem cells (hBMSCs) demonstrated that WH can enhance the proliferation and promote the osteogenic activity of stem cells in comparison with HAP. The as-synthesized WH using our novel reproducible and robust methods has great potential for future use in osteogenic tissue engineering.

Poster Presentation : **ANAL.P-108**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Zone-Fluidics-Based Fluorescence Detection System for On-Line Analysis of Cyanide in Water

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A zone-fluidics (ZF)-based fluorescence detection system has been developed for highly sensitive determination of cyanide in water. Cyanide determined by measuring a strongly fluorescent isoindole derivative produced by reaction of ortho-phthalaldehyde (OPA), and primary amine in basic solutions. The ZF-based fluorescence detection system consists of a reactor for OPA reaction, a detector, a light-emitting diode, an interference filter, and fluidic manipulation parts including a syringe pump, a multiport valve, and a tubing loop. In the tubing loop, sample, OPA, and glycine segments are separated by intervening air segments to prevent sensitivity decrease caused by mixing of fluid segments prior to the fluorescence detection. The ZF-based fluorescence detection system secures a linear response range of 5–250 μg/L ($R^2 = 0.9995$) and a low detection limit of 0.76 μg/L (S/N = 3).

Poster Presentation : **ANAL.P-109**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Thickness Measurements of Pharmaceutical Coatings using Hyperspectral Raman Spectroscopy

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The coating of pharmaceutical tablet not only improves surface properties of products but controls drug release time from the body. Therefore, degree of coating should be uniform, since it directly affects the human body. Although manufacturers attempt to coat all the tablets uniformly, it is difficult to control the coating thickness of all drugs completely because tablets have anisotropic structures and are coated in large quantities during the manufacturing process. In terms of quality control, process analysis techniques (PAT) with spectroscopic techniques are strong candidates for measuring coating thickness because they take advantage of fast detection capability, chemical selectivity and non-destructive. Previously, we study that we could correlate Raman spectra with thickness of outer layer by wide-depth hyperspectral SORS (W-SORS). In this study, we developed hyperspectral Raman line-mapping system capable of single shot analysis to monitor the coating thickness of pharmaceutical tablets. The key of hyperspectral Raman line-mapping system is the Raman intensity ratio between the coating substance and the inner pharmaceutical components, which is proportional to the coating thickness. We demonstrate that the hyperspectral Raman line-mapping system offered excellent calibration and prediction of the coating thickness of 270 acetaminophen tablets. In addition, we measured the absolute thickness of reference coating with confocal Raman system and could estimate the thickness of each tablet coating layer.

Poster Presentation : **ANAL.P-110**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Development of comprehensive analytical method of Persistent organic pollutants (POPs) in human serum by two different gas chromatography-mass spectrometry

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Persistent organic pollutants (POPs) are lipophilic substances that were ubiquitous in the environment and toxic to human such as Polychlorinated biphenyls (PCBs), Polybrominated diphenyl ethers (PBDEs) and organochlorine pesticides (OCPs). Due to their ability to bio-accumulate and potential for long-range transport, it is important to develop analytical method for quantitation at a very low level of POPs. In this study we applied the QuEChERs (Quick, Easy, Cheap, Effective, Rugged, and Safe) preparation method to reduce preparation time, effort, and the amount of sample. The method was validated and optimized, and the performance of ionization sources (atmospheric pressure chemical ionization and electron ionization) were compared. During the extraction step, some compounds such as PCB-18, PCB-28, PCB-44, PCB-52, PCB-49, pentachlorobenzen, and hexachlorobenzene were detected at a significant level in some polypropylene tubes so we selected the disposable tubes showing lowest background signal. Two different ion source showed significantly different sensitivity for many compounds, 63 compounds (73%) among total 87 target compounds were showed the lower method limits of detection (mLODs) that were 2-50 fold lower in APCI-MS/MS than GC-EI-MS/MS. Linearity was achieved in the region ($R2 \geq 0.99$) from each calibration curve both in APCI-MS/MS and GC-EI-MS/MS. These methods were also compared by performing analysis in 25 real human serum samples.This study was funded in part by the Korea Ministry of Environment (MOE) as ‘‘the Environmental Health Action Program. (project number: 2017001360003)’’ and in part by an intramural grant from Korea Institute of Science and Technology.

Poster Presentation : **ANAL.P-111**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

The optimized purification progression of mutations in melanocortin 4 receptor related to obesity for biochemical study.

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The human transmembrane protein (hTMP) including integral membrane protein have various functions like signal transduction, cell-cell recognition, anchorage and transport, etc. Among these crucial biological roles, human melanocortin 4 receptor (hMC4R) as G-protein coupled receptor (GPCR) are responsible for signal transduction related to regulation of metabolism and homeostasis. More specifically, hMC4R from pituitary gland helps us recognize when we are full in fed state by attachment with α-melanocortin stimulating hormone (α-MSH) matured in pro-opiomelanocortin (POMC) neurons. However, if 90th amino acid, aspartic acid located second transmembrane domain (TM2) is substituted to asparagine, function of receptor remarkably declines. Nearly complete loss of function in terms of agonist-stimulated signaling leads to appetite-control disorder, the reason of early on-set obesity. In order to demonstrate the functional deficiency between wt-hMC4R-TM2 and m-hMC4R-TM2, structural change should be identified because function of peptide is related to structure closely. Despite of importance of structural study, expression and purification of transmembrane protein composed of hydrophobic amino acids are challenging. Because membrane proteins are insoluble for aqueous solutions, the FPLC using sodium dodecyl sulfate (SDS) as a detergent which interferes with the various techniques used for characterization was used to isolate the target transmembrane proteins from impurities. After removing SDS, the obtained transmembrane protein was applied to various biophysical techniques like MS, CD, solution NMR spectroscopy, and solid-state NMR spectroscopy.

Poster Presentation : **ANAL.P-112**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Effective Sample Preparation of Polyphenols in Wine using Deep Eutectic Solvent-based Dispersive Liquid-Liquid Microextraction for HPLC-UV Determination

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Polyphenols are phytochemicals that exist in grapes and are beneficial to human health. In this study, resveratrol, oxyresveratrol and piceatannol in wine were extracted by deep eutectic solvent based on dispersive liquid-liquid microextraction (DES-DLLME), and a method for quantification these polyphenols using high performance piquid chromatograph - UV/Vis (HPLC-UV/Vis) was established. Several parameters for sample extraction, clean-up and concentration were optimized and verified by Central Composite Design (CCD) using Design Expert 11. The optimized sample preparation parameters are as follows: type and ratio of DES as extraction solvent, methyltributylammonium chloride / decanoic acid(1:3 molar ratio); type and volume of basic solvent, $KHCO_3$ and 1.3 mL; volume of acetic, anhydride, 250 μL; time of derivatization, 5min; type of dispersive solvent, methanol; ratio of extraction and dispersive solvent, 1:5.5; and salt 1.0 g. Chromatographic separation with HPLC/UV-vis was performed using Agilent HPLC 1100 series, ACME C_{18} (4.6mm id × 150 mm length, 5 μm particle size) column and gradient elution mode using water and 70% methanol. From the established extraction and HPLC-UV conditions, the limit of detection (LOD) and limit of quantitation (LOQ) of three analytes in the spiked sample were 6.09 - 11.77 μg/L and 18.47 - 35.66 μg/L, respectively. Recovery studies were performed at low, medium and high concentration range in calibration curve, and accuracy and precision in working range were 81.33 - 108.25 % and 2.03 - 10.73 RSD %, respectively. The calibration curves for the quantitative analysis were obtained the concentration range of 18.47 - 184.7 μg/L, 35.66 - 356.6 μg/L and 27.42 - 274.2 μg/L with correlation coefficient(r^2) from 0.9909 to 0.9984, respectively. The proposed method was applied to the determination of polyphenols in wine samples.

Poster Presentation : **ANAL.P-113**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Development and identification of biocompatible antimicrobial materials target sepsis from endophytic microbials

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This study aims to identify and develop antimicrobial substances that suitable for human body. Ninety six natural biological extracts were obtained from the culture broth of endophytic microbial. endophytic microbials were supplied from Korea Plant Resources Research Institute (KNIBR). Culture broths of endophytic microbial were extracted by liquid-liquid extraction in ethyl acetate and then concentrated samples were validated to identify antimicrobial activities using paper disk assay on sepsis-related pathogens including Escherichia coli (gram negative), Klebsiella pneumonia (gram negative), Staphylococcus aureus (gram positive), Enterococcus faecalis (gram positive), Streptococcus pseudopneumoniae (gram negative) and Candida albicans (yeast). Then, several whole extracts were validated that have excellent antimicrobial activities and here we focused on C10 sample to identify functional chemical compound within whole extract through fractionation using HPLC. Here we optimized fractionation conditions to distinguish various chemical compounds within the whole extract and all fractions were tested to validate the antimicrobial activity using paper disc assay. Their structure was characterized using by NMR and mass spectrometry-based analysis will be also performed in the future.

Poster Presentation : **ANAL.P-114**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Digital and Absolute Quantification of Microdroplets using Wide-Field Imaging System for real-time Droplet Sorting

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Droplet-based microfluidics (DMF) have been developed as a digital assay that allow precise and absolute quantification of targets such as enzyme, bacteria and nucleic acid. To avoid complex and expensive optic system as a detector, CCD sensors and smartphones have been integrated with DMF to image droplets. Here, we introduce digital CFU assay for absolute quantification of living-bacteria using 50.6-megapixel CMOS sensor which allow imaging the area of 10 cm2. Detectable number of droplets depends on the diameter of droplets, and it can be calculated as 9.29×106, 5.8×105 or 1.5×105 droplets when droplets are generated as 10, 40 or 80 μm in diameter, respectively. In this approach, 107 droplets can be analyzed within one minute after being generated and digital CFU assay was performed as a proof of concept study for the absolute quantification of living bacteria without fluorescent labeling. As a wide-field imaging system, 100 mm macro and full-frame 50.6-megapixel CMOS sensor-integrated digital camera were used to image droplets, and droplet images were analyzed using Matlab that simultaneously analyzes five individual colors. Bacterial cells (E.coli) were encapsulated within droplets as a single cell manner using microfluidic device and phenol-red was co-encapsulated as a pH indicator to detect living bacteria. In addition, we have investigated the migration of ammonia gas from bacteria and colorimetric dye between droplets. Interestingly, the dye was not able to across between the droplets but ammonia gas permeated through the droplets. Here, we introduce a detection platform (wide-field imaging system) that can be used for the monitoring large number of droplets (up to 107) within 5 minutes.

Poster Presentation : **ANAL.P-115**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Integration of Surface-enhanced Raman Scattering (SERS) with droplet digital PCR for the Monitoring *Klebsiella pneumoniae* at a single-cell sensitivity.

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Surface enhanced Raman Scattering (SERS) has been widely spread for monitoring chemical and biological analytes due to its potential of multiplexing ability and high sensitivity. However, the last requirement of reproducibility remains one of the biggest challenges in the SERS-related analytical fields where target concentration is extremely low.In this study, we described integration of SERS with PCR for the detection of *Klebsiella pneumoniae*. *K. pneumoniae* is a widely spread nosocomial pathogen. A rapid and sensitive detection method is required to guide therapeutic treatment of *K. pneumoniae* in clinical setups. It is also well-known as food-borne bacteria which precise monitoring is required in food industries. More specifically, silver (Ag) and gold (Au) hybrid nanoparticles were synthesized and Raman probe-conjugated DNA-based 'structure switching sensors' were immobilized on it. Then, *K. pneumoniae*-specific sequence was amplified with asymmetric PCR approach and it was detected using Ag-Au hybrid SERS sensors. Here, we demonstrated that single cell detection of *K. pneumoniae* using integrated PCR-based SERS and droplet-based microfluidics. This platform technology will provide a potential for multiplex monitoring of pathogens at a single cell sensitivity.

Poster Presentation : **ANAL.P-116**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Programmable paper-based microfluidic devices with printed patterns for analytical assays

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Regulating the flow of fluid in microfluidic devices enables a wide range of assay protocols for analytical applications. A programmable, paper-based microfluidic device fabricated by using a method of cutting and laminating, followed by printing, is reported. By printing silver-nanoparticle (AgNP) and poly[4,5-difluoro-2,2-bis(trifluoromethyl)-1,3-dioxole-co-tetrafluoroethylene] (PTFE) patterns on the surface of a paper channel, we were able to either increase or decrease the flow of fluid in the fabricated devices. By using hydrophilic AgNP patterns, we were able to increase the speed of fluid flow in the channel by up to 15 times compared to that in a pristine channel, and by using hydrophobic PTFE patterns, we were able to delay that speed by a factor of about 3. Using the programmable, paper-based microfluidic device, we demonstrated a single-step protocol for detecting glucose and a multi-step protocol for detecting methyl paraoxon (MPO). We anticipate that our programmable, paper-microfluidic device will lead to improved fluid handling techniques, which are crucial for achieving a wide range of analytical assays.

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Poster Presentation : **ANAL.P-117**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Highly Sensitive Chemiluminescent Probe for Dectecting NQO1 Levels in Cancer Models

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Activatable (turn-on) probes that permit the rapid, sensitive, selective, and accurate identification of cancer-associated biomarkers can help drive advances in cancer research. Here we report a smart novel NAD(P)H:quinone oxidoreductase-1 (NQO1) specific chemiluminescent Probe 1 that allows the differentiation between cancer subtypes. Probe 1 incorporates an NQO1-specific trimethyl-locked quinone trigger moiety covalently tethered to a phenoxy-dioxetane moiety through a para-aminobenzyl alcohol linker. Bioreduction of the quinone to the corresponding hydroquinone initiates a series of steps, which result in a chemiluminescent signal. As inferred from a combination of in vitro cell culture analyses and in vivo mice studies, the probe is safe, cell permeable, and capable of producing a ‘turn on’ luminescence response in an NQO1-positive A549 lung cancer model. No such signal output was observed in an NQO1-negative H596 lung cancer model. On this basis we suggest that Probe 1 can be used to identify cancerous cells and tissues characterized by elevated NQO1 levels

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Poster Presentation : **ANAL.P-118**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

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

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Lipids are main components of cell membranes which are involved in various cellular functions and play an essential roles in biological system such as energy storage and cell signaling. Lipid metabolism is a dynamic biological process that includes lipid synthesis, accumulation, distribution to various specific tissues and excretion. Lipidomics is the large-scale study of lipid metabolism such as pathways and networks of lipids in biological system and approach to investigate the qualitative and quantitative profile of the lipid components. In recent, lipidomics has become a significant tool in a diverse research field such as biomarker discovery related to diseases, foodomics, and microbiomes and probiotics. In order to accomplish accurate lipidomic analysis, it is necessary to analyze a large number of samples at a high speed and high throughput separation condition for nanoflow ultrahigh performance liquid chromatography (nUHPLC) covering broad lipid classes without spectral congestions in the MS detection. In this study, a high-throughput and rapid lipid analysis can be carried out within 10 minutes by adjusting gradient elution conditions without incurring the spectral complexity. The time-based plate number (N/t) which represents the time dependent efficiency of a separation condition is maintained with 10 minutes of gradient elution compared to a typical 20 min of separation.

Poster Presentation : **ANAL.P-119**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Global analysis of polyglycerophospholipids using isotope-labeled methylation and nUHPLC-ESI-MS/MS

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Polyglycerophospholipids (PGPLs) are phospholipids (PLs) with multiple glycerol moieties synthesized from phosphatidylglycerol (PG) as a common precursor. PG, Bis(monoacylglycero)phosphate (BMP), bis(diacylglycero)phosphate (BDP), and hemi BDP have two glycerols and cardiolipin (CL), monolysocardiolipin (MLCL), and dilysocardiolipin (DLCL) have three glycerols. Since they are closely related to each other and regarded as biomarkers with high selectivity in various diseases rather than other PLs, simultaneous analysis of PGPLs is important to understand their pathological roles. In this study, isotope-labeled methylation (ILM) method with nUHPLC-ESI-MS/MS was utilized for relative quantitation of PLs without the addition of internal standard lipids. The molecular structures of methylated PGPLs were identified by collision induced dissociation (CID) experiments. The efficiency of methylation for PGPLs was found to be higher than 97% and the S/N ratio of most species was improved including newly identified species (regioisomers of Hemi BDP, DLCL, and MLCL). LOD values were ranged from 2.92 for MLCL (18:2)3 to 21.38 fmol for PG (14:0)2, which were much higher than those without methylation. When SH-SY5Y cells with and without the drug treatments to induce Parkinson's disease model were analyzed, a total of 229 PGPLs including 11 PG, 9 BMP, 16 Hemi BDP, 1 BDP, 71 MLCL, 121 CL species were identified, which are the highest number reported so far. Furthermore, seven CL species having arachidonic or docosahexanoic fatty acid chains were found to increase upon drug treatment, which is an indicative of CL remodeling process in Parkinson's disease.

Poster Presentation : **ANAL.P-120**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Separation of exosomes and lipoproteins in human serum using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

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Exosomes play an important role in maintaining homeostasis and intercellular communication in body fluids and are known to be associated with physiological and pathological functions. Recently, exosomes are expected as a biomarker for disease prognosis and diagnosis. In particular, a number of studies have shown that blood exosomes are closely related to cancer. Lipoproteins carry lipids through the blood stream and are classified according to its size and density. Because of the similarity in their size and density of lipoproteins, it is important to separate exosomes and lipoproteins from bloodField-flow fractionation (FFF) is an analytical technique that is capable of separating nano to micron sized particles in an aqueous solution in an empty channel space without packing materials. In this study, exosomes and lipoproteins in human serum were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) using field programming and monitored by a series of UV and multi-angle light scattering (MALS) detectors. During separation, fractions of exosome and lipoprotein were collected and analyzed by Western blot, transmission electron microscope (TEM), and nUPLC-ESI-MS/MS for proteomic.

Poster Presentation : **ANAL.P-121**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Size fractionation of Graphene Oxide by Asymmetrical Flow Field-Flow Fractionation

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Graphene is known to have surprising properties including electrical, thermal and mechanical properties. However, graphene still has many problems with applications on the market, because of low solution dispersibility and poor processability. To solve these problems, graphene oxide liquid crystal (GOLC) was discovered. In contrast to graphene, GOLC is a two-dimensional graphene-based material that has a good processability at large scales and is well dispersed due to the liquid crystal characteristics, therefore, it is expected to be utilized for the various applications. However, GO has a wide size distribution due to various factors in the synthesis step. GO size distribution needs to be controlled because it relates to the liquid crystal characteristics of GO. Many studies have been conducted to solve the problem of wide size distribution of graphene oxide, but it has not been solved effectively yet. These studies pose problems with size separations that modify graphene oxide. This study was aimed to find an optimal condition for the size-based separation of GO using asymmetrical flow-field fractionation (AF4). For the confirmation of size separation, fractions GO were collected and analyzed using scanning electron microscopy (SEM) and optical microscopy (OM). As a result, GO in plate form can beseparated by hyperlayer separation mode of AF4 with the recovery of GO within 70% to 90%.

Poster Presentation : **ANAL.P-122**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Lipidomic alterations in lipoproteins of patients with postmenopausal osteoporosis by asymmetrical flow field-flow fractionation and nUHPLC-ESI-MS/MS

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As aging population increases, osteoporosis is becoming an worldwide issue. Pathological mechanism of osteoporosis is unclear, but osteocytes affected by oxidized lipids are expected to be a major factor. Lipids play important roles in signal transmission and various cellular processes. Therefore, it is important to study relationships between lipids consisting lipoproteins in plasma and osteoporosis for the detection of osteoporosis at the early stage. There were previous studies about lipids and osteoporosis in medical field but none of them conducted quantitative and qualitative analysis at the molecular level in detail.In this study, 20 postmenopausal female plasma samples were classified into the groups of patients in which women having osteoporosis with no medical history (n=10), and age-matched control(n=10). Flow field-flow fractionation (FlFFF) is an elution-based separation technique that can sort particles or macromolecules by sizes. FlFFF analysis of patient's plasma resulted inshowed that the relative levels of low-density lipoprotein (LDL) of the patient groups were higher than those of the control with the increase in retention time, while those of high-density lipoprotein (HDL) from patients were not significantly altered compared to those of control. Lipids in lipoprotein fractions collected during FlFFF runs were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). Overall, 379 lipids from patient's plasma were identified and 252 lipids were quantified. With statistical evaluation, 21 lipid species (6 PC, 3 PEp, 4 HexCer, 2 TG and 1 each from LPA, PA, LPI, PI, SM, Cer) were found to show significant changes (> 1.5 fold and $p < 0.05$) in comparison to healthy controls.

Poster Presentation : **ANAL.P-123**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Optimizations in simultaneous analysis of free fatty acid and other lipid classes using nUHPLC-ESI-MS/MS

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Lipids are the signaling molecules to affect metabolism. Perturbations in lipid profiles of phospholipid (PL), glycerolipid (GL), sphingolipid (SL), and free fatty acid (FFA) are closely associated with the development of metabolic diseases such as diabetes mellitus and cardiovascular disease. When analyzing FFA from lipidome from plasma or tissues by liquid chromatography with electrospray ionization mass spectrometry (LC-ESI-MS), retention of FFA often overlaps with lysophospholipids (LPL) due to their similar nature in polarity. Moreover, if FFA is dissociated from other lipids containing acyl chains when they are introduced to MS, analysis of FFA can be disturbed.This study was focused to optimize run conditions of analyzing FFA with other lipid classes by nanoflow ultrahigh pressure LC-ESI-MS/MS (nUHPLC-ESI-MS/MS). Modifiers of 0.5 mM ammonium formate and 0.05% ammonium hydroxide were optimized for simultaneous analysis of FA and other lipid classes. When ESI voltage and heated ion transfer tube temperature were examined to determine the effect of unintended in-source fragmentation (ISF), the analysis of FFA was not disrupted by ISF of other lipid classes. ESI voltages of 1.5 (negative) and 3 kV (positive), and heated ion transfer tube temperature of 350 °C were optimized for both precursor intensity and generation of ISF. When extraction efficiencies of several extraction methods were examined for extraction of FFA of plasma from mice, extraction method using MTBE/MeOH was found to be optimal. Optimized conditions were applied to examine lipid profiles of plasma from mice and 330 lipid species including 26 FFAs were identified based on collision-induced dissociation (CID).

Poster Presentation : **ANAL.P-124**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Investigation of serum lipid signatures of pig in post-hepatectomy liver failure from expanded hepatectomy using nanoflow UHPLC-ESI-MS/MS

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The liver is an important organ that is involved in numerous biochemical reactions andlipid metabolism. Because the liver is an excellent regenerative organ, liver resection is usually performed when liver cancers were developed. However, hepatectomy may cause a variety of complications. The biggest contributor to mortality from liver resection is a post-hepatectomy liver failure (PHLF) which is the inability of the liver to perform its normal synthetic and metabolic functions after liver resection. Therefore, an early and quick diagnose of PHLF is still an important issue.In this experiment, pigs were divided into three groups of six laparotomized pigs (sham), seven 70% partial hepatectomized pigs (the 70% PH group), and seven 90% partial hepatectomized pigs (the 90% PH group) to obtain sera at each time points: pre-operation (PO), 14 hours (14h), 30 hours (30h), and 48 hours after the operation. The lipids extracted from sera were analyzed using nanoflow ultrahigh-pressure liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS) and 284 lipid species were structurally confirmed by collision-induced dissociation (CID) experiments. Among them, 184 lipid species were quantified by selective reaction monitoring (SRM) mode. From the statistical analysis, eleven lipids showed significant differences (> 2-fold, $p < 0.01$) between the 70% and the 90% PH groups at 30 hours after the operation. Among the lipids, TG was decreased considerably at 90% PH. PC plasmalogen was increased at 90% PH and showed significant correlation (Pearson’s $r > 0.7$, $p < 0.05$) with total bilirubin (TBIL) and prothrombin time (PT) which indicate liver function.

Poster Presentation : **ANAL.P-125**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

NMR study of human transmembrane proteins related to disease

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Human transmembrane proteins (hTMPs) are the type of integral membrane proteins and act as a gatekeeper to regulate the movement of materials such as ions, hormones, and signaling molecules into and out of cells. But, 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. To understand the mechanism and function of hTMPs, it is critical to elucidate the three-dimensional structure of them. In this study, we tried to identify the structure of syndecans-4 (Syd4) receptor and human amyloid precursor transmembrane protein (hAPP-TM). Syd4 is transmembrane heparan sulfate proteoglycan (HSPG) belonging to the syndecan family and has a common basic structure including extracellular domain, transmembrane domain and cytoplasmic domain. It may influence tissue development and repair as well as the pathogenesis of numerous diseases like cancer. We demonstrated methods that optimized for recombinant expression and purification of three kinds of Syd4 such as cytoplasmic and short extracellular domains of Syd4 (Syd4-eTC), wild type Syd4 (wt-Syd4), and mutant Syd4 (m-Syd4). The hAPP, which is known as the precursor molecule whose proteolysis generates hAβ (human amyloid-β), related Alzheimer’s disease. One of the possible mechanisms for hAβ toxicity suggests that form calcium-permeable ion channels and these channels might allow excessive calcium influx and disrupt the cellular calcium homeostasis. We optimized expression and purification methods and characterized them using various biophysical techniques like MS, CD, solution NMR, solid-state NMR spectroscopy. In addition, we used solution NMR, and solid-state NMR spectroscopy to identify structural of hTMPs.

Poster Presentation : **ANAL.P-126**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Wavelength-Dependent Defocused Imaging of Single Gold Nanorods under Three-Color Total Internal Reflection Scattering Microscopy

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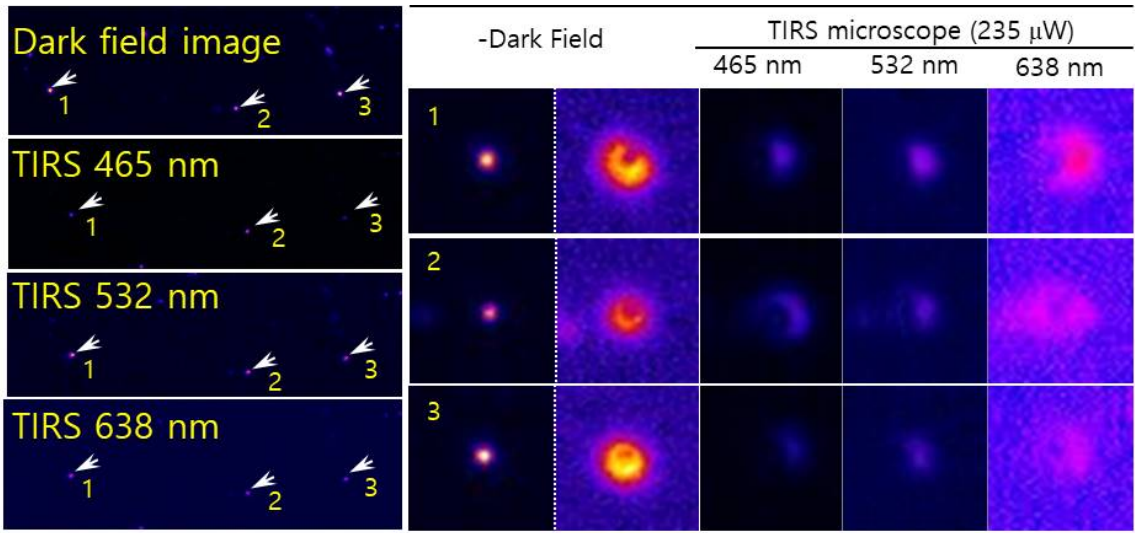
Localized surface plasmon resonance (LSPR) refers to the collective oscillations of conduction band electrons in noble metal nanoparticles, which are induced by the time-dependent electric field of an electromagnetic wave. The LSPRs of noble metal nanoparticles have been well known to be strongly dependent on the particle size, shape, surrounding dielectric environment and proximity to other nanoparticles (plasmon coupling). In this study, we investigated the plasmonic anisotropic properties of single gold nanorod (AuNR) using a three-color total internal reflection scattering (TIRS) microscope and a scanning electron microscope (SEM). The spatial scattering field distributions of single AuNRs were revealed by a defocused imaging technique under TIRS microscopy equipped with three-different lasers of 465 nm, 532 nm and 638 nm. The scattering signals and spatial orientations were analyzed in the defocused state to confirm the 3D orientations of single AuNRs deposited on the glass substrate. Finally, we further compared the 3D orientations (or spatial field distributions) of single AuNRs obtained from conventional dark-field (DF) microscopy. Therefore, this study provides a deeper understanding of the spatial field distributions of single anisotropic AuNRs under TIRS geometry equipped with three different colors.


Dark field image
1
2
3
TIRS 465 nm
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TIRS 532 nm
1
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TIRS 638 nm
1
2
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-Dark Field
TIRS microscope (235 µW)
465 nm
532 nm
638 nm
1
2
3

Poster Presentation : **ANAL.P-127**
Analytical Chemistry
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Reducing Process of Silica Particle by Metallothermic Reduction Reaction

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Recently, metallothermic reduction reactions (MRRs) are displacement reactions that use reactive metals to reduce nonmetal materials, mainly silicon and carbon, particularly in their nanostructured forms obtained using an MRR with magnesium as the reductant. Here, we mixed magnesium/aluminum with anisotropic Au@SiO2 core-shell nanoparticles and heated it up to 650℃ to reducing silica shell. We found that small parts scattered in the silica shell were found to be converted to silicon with crystallinity in early time in the heating process. And the reaction progresses, it became porous silicon shell with anisotropic gold nanoparticles as a core structure. It shows that reduction reaction starts inside the silica particle such as island and it proceeds to around. Finding the optimal conditions, this core-shell nanoparticle could be used for dual imaging in bio-healthcare applications.

Poster Presentation : **ANAL.P-128**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Viscoelastic Nanocomposites with Boron Nitride in Polymer Matrix

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BNNTs nanocomposites have attracted great attention in a variety of application including electronics, aerospace, biomedicine and nuclear safety because they have great thermal, electrical, mechanical properties and neutron shielding effect and biocompatibility. We fabricated cost-competitive and scalable viscoelastic boron nitride nanotubes (BNNTs) nanocomposites using eutectic liquid (EL) and polymer matrix. EL combining two simple chemicals simply, has been mixed with polymers such as polyurethane and epoxy resins. In addition, we report the thermal and electrical conductivity of this nanocomposites.

Poster Presentation : **ANAL.P-129**
Analytical Chemistry
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Control of Desired Aspect Ratio of Gold Nanorods based on Seed-Mediated Method.

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Seed-mediated method is a general procedure for the synthesis of gold nanorods(Au NRs) who developed Murphy et al. and El-Sayed et al. Many of the interesting optical properties of Au NRs are determined by the position of their LSPR peak, which is largely governed by the aspect ratio of Au NRs. In this experiment, we have controlled parameters to tuned from visible to infrared by tuning their aspect ratio. As a result, we show the tunable plasmon bands depending on the volume/concentration of the chemical reagents by using hydroquinone as a reducing agent in the presence of silver nitrate and the longitudinal LSPR peak is still in the range of Vis-NIR even if the size of Au NRs is less than 20nm in length. And previously known LSPR peaks of Au NRs are less than 900nm or more than 1200nm. But we also synthesize high aspect ratio Au NRs with peaks more than 1,200nm by using co reducing agent.

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Poster Presentation : **ANAL.P-130**
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Electrochemical Immunosensor using Nanotriplex of Graphene Quantum Dots, Fe3O4, and Ag Nanoparticles for Tuberculosis

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

Poster Presentation : **ANAL.P-131**
Analytical Chemistry
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Performance evaluation of SERS-PCR sensors for future use in rapid and sensitive genetic assays

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Herein, we report a surface-enhanced Raman scattering (SERS)-based polymerase chain reaction (PCR) assay platform for the sensitive and rapid detection of a DNA marker (pagA) of Bacillus anthracis. Real-time quantitative PCR (RT-qPCR) has been recently considered a gold standard for the quantitative evaluation of a gene expression level but it still suffers from the problem of a long thermocycling time. To address this issue, we developed a conceptually new SERS-PCR platform, and evaluated its performance by sequentially measuring the Raman signals of Bacillus anthracis DNA after the completion of different thermocycling numbers. According to our experimental data, SERS-PCR has lower limit of detections (LODs) than RT-qPCR under the small cycle number of 20. In particular, it was impossible to detect a target DNA amplicon using RT-qPCR before the number of cycles reached 15 but SERS-PCR enabled DNA detection after only 5 cycles with a LOD value of 960 pM. In addition, the dynamic range for SERS-PCR (0.1–1,000 pM) is wider than that for RT-qPCR (150-1000 pM) under the same condition. We believe that this SERS-PCR technique has a strong potential to be a powerful tool for the rapid and sensitive diagnosis of infectious diseases in the near future.KEY WORDS: SERS-PCR assay, low PCR cycle, Bacillus anthracis,

Poster Presentation : **ANAL.P-132**
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Functionalization of gold nanoparticles using guanidine thiocyanate for sensitive and selective visual detection of Cd^{2+} ion

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AbstractSoil, air, and water are immensely polluted as a result of the advancement of the chemical and farming industry. Moreover, it can be accumulated easily in a human body via food chains, which is hazardous for human health. Cadmium heavy metal extensively used in the Ni-CD battery, cadmium pigments and stabilizers and cadmium composites [1]. When the amount of Cd^{2+} ion reaches beyond 3 μg/mL in a human body, it will begin to combine with DNA and initiate to denaturation of proteins [2]. Thus, there is a need for highly selective and sensitive on-site detection system for Cd^{2+} ion. Herein, a simple synthetic approach has been developed for the identification of Cd^{2+} ion dependent on surface modification of gold nanoparticles (AuNPs) using guanidine thiocyanate (GT). GT contains guanidinium cation and thiocyanate anion, which can form self-assembled monolayer on AuNPs. Moreover, the negative charge on the GT surface provides a repulsive force that prevents the self-aggregation of AuNPs by modifying the surface. The as synthesized GT-AuNPs is utilized as a probe with excellent sensing ability and high sensitivity for the target analyte. The limit of detection found to be 10 nM by UV-visible spectroscopy for Cd^{2+} ion. The real-world applicability of the scheme was evaluated by investigating Cd^{2+} ion in water samples, signifying its feasible application in environmental water and food sample analysis.**Keywords**: Cd^{2+} detection, colorimetric sensor, UV-visible spectroscopy, GT-AuNPs**Reference**1)D. M. Templeton, Y. Liu, Multiple roles of cadmium in cell death and survival, Chem. Biol. Interact., 188 (2010) 267-275.2)F. Mo, Z. Ma, T. Wu, M. Liu, Y. Zhang, H. Li, S. Yao, Holey reduced graphene oxide inducing sensitivity enhanced detection nanoplatform for cadmium ions based on glutathione-gold nanocluster, Sensors Actuat B. Chem., 281 (2019) 486–492.

Poster Presentation : **ANAL.P-133**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Advanced studies of antimicrobial peptides derived from bovine milk with structural analysis using NMR

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Nowadays bacteria that have Anti-Microbial Resistance (ARM) are increasing due to antibiotics abuse. It has attracted people’s attention to antimicrobial peptides (AMPs). So we study LPcin-I and LPcin-II derived from lactophoricin, a cationic amphipathic antimicrobial peptide consisting of 23 amino acids. Here we found that antimicrobial activity in the polypeptide is related to the N-terminal, not the C-terminal and tried to use this point to develop commercially efficient antimicrobial peptides. 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 improve AMPs with a shorter length. First, the serine located in the hydrophilic part was mutated to lysine to increase the net charge. Next, amphipathicity was reduced to prevent self-aggregation. Finally, tryptophan was added to facilitate interaction with the bacterial membrane. Therefore, we designed and confirmed the new antimicrobial peptides YK5, YK8 and YK11 based on YK3.We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with many biophysical techniques. We performed MALDI-TOF MS and CD spectrometry for structure refinement. In order to investigate the structures and dynamics, we use various 1D and 2D NMR techniques using micelle and especially bicelle samples to mimic membrane environments. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra.

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Poster Presentation : **ANAL.P-134**

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Fluorescent Displaying Time-dependent Iron selenide Quantum dots

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Fluorescence from nanoparticles quantum dots have stimulated considerable interest because of their unique and useful optical properties. The fluorescence wavelength at the QDs depends on the size of the particles, even if it consists of the same material. The smaller the particle size, the shorter the wavelength, and by adjusting the size, the more fluorescence in the visible light domain of the desired wavelength can be produced. Here, one-pot synthesis of water-soluble fluorescent iron selenide(FeSe) is demonstrated to be an increase in the size of particles over the reaction time. Moreover, the fluorescence intensity is clearly different over the reaction time. The sample with the longest response time display fluorescence more clearly at an excitation wavelength of 365nm. UV-vis spectrum and other optical measurements such as PL-spectrum reveal the growth of FeSe.Availability of one-pot synthesis of water-soluble Fluorescent FeSe is expected to stimulate further studies of these materials in chiral quantum dots.

Poster Presentation : **ANAL.P-135**
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NMR structural studies of tIK fragment with anti-inflammatory effective

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Rheumatoid arthritis is caused by an autoimmune disorder. Various immune cells such as T cells, B cells, macrophages and dendritic cells participate in the inflammatory response of RA. Initially, inflammation starts around the synovial membrane around the joint, spreading around cartilage, ligaments, and destruction. In addition, inflammation of the blood vessels and skin may lead to systemic diseases such as vasculitis, anemia, and headache. There are many causes for the disease, but one of them is known as the imbalance of pro-inflammatory cytokines and anti-inflammatory cytokines. In addition, self-antigen recognition due to abnormal major histocompatibility complex (MHC) class II-expressing B cells produces antibodies that induce more severe RA. Recent studies have showed that truncated-IK (tIK) protein`s derivatives downregulate MHC class II on activation in inflammatory diseases. Therefore, we conducted epitope research to develop tIK as a new anti-inflammatory therapeutic agent for rheumatoid arthritis patients. In our study, we examined the phosphorylation pattern of protein cell signaling by isolating macrophages from transgenic mice transplanted with the tIK nucleotide sequence. It has been reported that tIK protein phosphorylates the 496th tyrosine of interleukin 10 receptor subunit alpha and has anti-inflammatory effect. We sought to find tIK protein’s specific regions that induce phosphorylation at the interleukin 10 receptor subunit alpha. So, we predicted the possible structure of tIK based on IL-10 through sequence homology modeling and proposed 4 anti-inflammatory peptide candidates and identified the anti-inflammatory activity through the TH17 cell differentiation test. Among them, the 18-mer peptide with anti-inflammatory activity was named tIK-YK4. Afterwards, we found 9-mer and 14-mer, based on 18-mer, and anti- inflammatory effect was also confirmed. Currently, we have successfully performed overexpression using E. coli and are optimizing the purification process. And we are trying to identify the relationship between structure of these peptides and anti-inflammatory activity through NMR studies.

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Ultrathin multi-functional NiCoFe/Ni nanostructured electrocatalyst for water-splitting

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Among the clean energy conversion technologies, hydrogen production through electrochemical water splitting ($2H_2O \rightarrow 2H_2 + O_2$) is one of a promising generation of green and renewable energy source. Water-splitting technologies depend on a series of electrochemical reactions such as oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). One of the main problems for the overall efficiency of water splitting is the sluggish kinetics of OER, which involves multiple steps of proton-coupled electron transfer. Theoretically, the minimum energy required to the catalytic decomposition of water is $\Delta G = 237.1$ KJ, that corresponds to an applied voltage of 1.23 V to overcome the thermodynamic energy barrier. To defeat the kinetic barrier at a relatively low overpotential, cost-effective and highly efficient catalysts are required. Here we report synthesis of ultrathin NiCoFe nanosheet through electrodeposition on nickel foam. Owing to its defect enriched structure with higher electrochemically active surface area, this NiCoFe nanosheet supported on Nickel Foam facilitate the diffusion of gaseous product (H_2 and O_2) and exhibited remarkable catalytic performance and outstanding stability for both HER, OER and also for overall water splitting in alkaline electrolyte.

Poster Presentation : **ANAL.P-137**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Photoluminescence enhancement by Ag@Fe3O4 nanoparticles

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Nanostructures with noble metals can enhance the photoluminescence because of confined strong electric field on the surfaces. Ag@Fe3O4 core/shell nanoparticles (NPs) have unique property, surface plasmon resonance (SPR), caused by silver core. This nanoparticles can be synthesized by one-pot hydrothermal method. Quantum dots (QDs) are nanoparticles made of semiconductor materials. Because of confined structure it has wide bandgap which can be tuned by changing the size of QDs. When the QDs are illuminated by UV light, an electron in the QDs can be excited to a state of higher energy. The excited electron can drop back into the state of lower energy by the emission of light. FeSe QDs are cardmium free material that more echo-friendly. Moreover it has photoluminescent and magnetic property in one body. But has lower quantum yield (QY) than other QDs such as CdSe, InP. Thus, we investigated the enhancement of photoluminescence (PL) from FeSe QDs by exciton-plasmon interaction and demonstrated that Ag@Fe3O4 NPs makes the low QY of FeSe QDs enhanced. Therefore, we expected that this experiment can develop the surface plasmonic excitation.

Poster Presentation : **ANAL.P-138**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of viral-magnetic hybrid Janus nanoparticles

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Janus nanoparticles (JNPs) are unique building blocks which have asymmetric structures. Typical silver nanoparticles which are spherical shapes, for example, are composed of silver themselves and surface is homogeneous. However, JNPs are formed by heterogeneous surface; half of side is different from another side. They have been attracted and studied because of their different chemical or physical properties. For instance, their asymmetry give chiral properties. When we synthesis JNPs using magnetic nanoparticles (MNPs), they are able to be arrayed in magnetic field. Asymmetry and magnetic properties offer efficient and distinctive methods to target complex self-assembled materials. Here, we made Janus magnetic nanoparticles with Fe3O4. We coated half of surface with gold through sputtering followed by coordination of M13 bacteriophages and made them be arrayed by magnetic field. JNPs we made seem shuttlecock shapes. To figure out optical properties of nanochains, UV-vis spectroscopy, Raman spectroscopy, and Fourier transform infrared spectroscopy (FTIR) are used. The unique optical properties of suprastructures of JNPs can be applied into color sensors, biosensors, and display research fields.

Poster Presentation : **ANAL.P-139**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Enrichment of phenolic compounds using PTAD functionalized particles

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Phenolic compounds are common constituents of various foods, beverages and plant tissues, and mostly act as antioxidants. They consist of aromatic rings with one or more hydroxyl groups that are known to be related to the antioxidant capabilities – reducing the diseases associated toxic effects stemming from reactive oxygen species and oxidative stress. In this poster, we introduce an efficient enrichment and detection method based on PTAD (4-phenyl-3H-1,2,4,-triazole-3,5(4H)-diones), which selectively reacts with phenolic compounds at the α position of the phenolic hydroxyl group to form a covalent carbon-nitrogen bond. We prepared disulfide-containing PTAD-presenting particles that can effectively and selectively enrich small amount of phenolic compounds in biological samples. The enriched phenolic compounds were then released from the solid support through disulfide cleavage, and subsequently analyzed by mass spectrometry (MS). MS analysis afforded the molecular weights of the enriched phenolic compounds without complicated protocols and reagents, and therefore, enabled multiplexed detection of several phenolic compounds. As a further work, we are currently expanding our strategy to the quantitative analysis of phenolic compounds in mammalian cells and animal tissues

Poster Presentation : **ANAL.P-140**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Application of SERS active AuNPs-MOF nanocomposite for sensitive detection of MGITC

Anupam Das, Namhyun Choi[1], Kyoung Neon Kim, Jaebum Choo*

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The current project is aimed to investigate the Surface-Enhanced Raman Scattering (SERS) properties of a nanocomposite (AuNPs-MOF) of gold nanoparticles (AuNPs) and Metal (Fe) Organic Framework (MOF), MIL-101(Fe)-NH2. Upon finding the SERS activity of the AuNPs-MOF nano composite, we found its applications in detecting trace amount of target protein transferrin (Tf) in spiked phosphate buffer saline (LOD: 1 nmol) and human serum (LOD: 0.625 μmol) samples. It was observed that upon increasing Tf concentration, overall SERS intensity of AuNPs-MOF-Tf complex gets enhanced significantly. Eventually, we established a calibration curve (SERS intensity vs Concentration of Tf) to find out the Total (or Transferrin) Iron Binding capacity (TIBC) values of unknown samples. Considering the normal TIBC level (~1.7 to ~3.7 g/L) of a healthy human being, we can calculate the TIBC value of given samples. TIBC values indicate whether the patients are suffering from iron deficiency.KEYWORDS: Surface-Enhanced Raman Scattering (SERS); SERS-active nanocomposite, Transferrin

Poster Presentation : **ANAL.P-141**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Functionalization of gold nanoparticles using guanidine thiocyanate for sensitive and selective visual detection of Cd^{2+} ion

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Soil, air, and water are immensely polluted as a result of the advancement of chemical and farming industry. Moreover, it can be accumulated easily in a human body via food chains, which is hazardous for human health. Cadmium a heavy metal, extensively used in the Ni-CD battery, cadmium pigments and stabilizers and cadmium composites [1]. When the amount of Cd^{2+} ion reaches beyond 3 μg/mL in a human body, it will begin to combine with DNA and initiate to denaturation of proteins [2]. Thus, there is a need for highly selective and sensitive on-site detection system for Cd^{2+} ion. Herein, a simple synthetic approach is developed for the identification of Cd^{2+} ion dependent on surface modification of gold nanoparticles (AuNPs) using guanidine thiocyanate (GT). GT contains guanidinium cation and thiocyanate anion, which can form self-assemble monolayer on AuNPs. Moreover, the negative charge on the GT surface provides a repulsive force that prevents the self-aggregation of AuNPs by modifying the surface. The as synthesized GT-AuNPs is utilized as a probe with excellent sensing ability and high sensitivity for target analyte. The limit of detection found to be 10 nM by UV-visible spectroscopy for Cd^{2+} ion. The real-world applicability of the scheme was evaluated by investigating Cd^{2+} ion in water samples, signifying its feasible application in environmental water and food sample analysis.**Keywords**: Cd^{2+} detection, colorimetric sensor, UV-visible spectroscopy, GT-AuNPs**Reference**1)D. M. Templeton, Y. Liu, Multiple roles of cadmium in cell death and survival, Chem. Biol. Interact., 188 (2010) 267-275.2)F. Mo, Z. Ma, T. Wu, M. Liu, Y. Zhang, H. Li, S. Yao, Holey reduced graphene oxide inducing sensitivity enhanced detection nanoplatform for cadmium ions based on glutathione-gold nanocluster, Sensors Actuat B. Chem., 281 (2019) 486–492.

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Poster Presentation : **ANAL.P-142**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

An investigation on the change of inorganic arsenic concentration in Hiziki by the pretreatment method using IC-ICP-MS

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The accurate determination of a toxic element in food has been important for the assessment of food safety. Accordingly the method for the reduction of toxic element in food also has been needed. Arsenic is well known as an element with high toxicity, but its toxicity depends on the chemical forms. Inorganic arsenic is more toxic than organic arsenic, thus the quantitation of inorganic arsenic in a food is critical. In particular, HIziki has been known to contain the inorganic arsenic. In this study, the determination of inorganic arsenic in Hiziki was performed, then the change of the concentration of inorganic arsenic was investigated with the various pretreatment methods of Hiziki. The inorganic arsenic was separated by ion chromatography (IC), then detected by inductively coupled plasma mass spectrometry (ICP-MS). The different pretreament methods were the soaking, steaming, and boiling the Hiziki. The concentrations of inorganic arsenic in Hiziki were reduced to 50%, 30%, 74% of the original concentration by soaking, boiling, and steaming, repectively.

Poster Presentation : **ANAL.P-143**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Micro headspace extraction for chlorophenols

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For the headspace (HS) extraction, analytes are evaporated from a donor solution to a vapor then extracted into an acceptor phase placed in the vapor. The extraction efficiency is obtainable when the analytes are transferred into the small acceptor phase and enrichment factor is given by volume ratio between the donor and acceptor phases. Therefore, a small acceptor phase volume and small vapor space are preferable. Herein, we present a new technique as a small bubble is performed in a capillary tip and opened connect to the capillary tube which contain a very small acceptor phase. A bubble is perfect hangable in the capillary inlet by the capillary hydrophobic tip which coated by a hydrophobic coating solution. Analytes evaporated into the bubble are extracted to the acceptor inside the capillary tube and finally the analytes are separated by normal capillary electrophoresis (CE). To improve bubble generation reproducibility and stability, capillary pretreatment method with strong alkaline solution (KOH) was confirmed. And optimized bubble volume was 100 nL, pH of donor phase was 3. Other parameters such as extraction time, temperature will be evaluated. This novelty technique is a quite convenient HS extraction in-line coupled with CE in an automatic process, be a most straightforward, inexpensive and sophisticated apparatus but providing a very high extraction efficiency, high sensitivity and be useful for numerous applications for the analysis of chlorophenols compounds in biological samples.

Poster Presentation : **ANAL.P-144**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Plasmonic Sensing of Pyridine by Chemical Interface Damping of Single Au/Ag Core Shell Nanorods.

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Noble metal nanoparticles have a unique optical property resulted from localized surface plasmon resonance (LSPR). In this study, we observed that the thicker the silver coated in Au/Ag core shell nanorods, the broadener the line width of LSPR under dark-field scattering microscopy and spectroscopy. The chemical interface damping (CID) is one of the plasmon decay processes in gold nanoparticles. Herein, to find new plasmonic metal that can induced CID as an alternative to gold nanorods, we conducted an dark - field (DF) scattering studids of Au/Ag core shell nanorods with pyridine as adsorbate. We investigated the CID induced by a pyridine attached on the Au/Ag core shell hybrid nanorods under dark-field scattering microscopy and spectroscopy. By the adsorption of pyridine molecules on the Au/Ag nanorods, their LSPR linewidth was broadened with decreasing the scattering intensity due to CID effect.

Poster Presentation : **ANAL.P-145**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Detection of the norovirus using magneto-plasmonic film

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The virus is usually spread by the facal-oral route. This may be by contaminated food or water or person-to-person contact. It may also spread via contaminated surfaces or through the air. Especially, norovirus results in about 685 million cases of disease and 200,000 deaths globally a year. It is common both in the developed and developing world. Confirmatory testing before get infected is so important. Here, we introduce a rapid and convenient sensing kit using magnetic-plasmon glass film (MagPlas film) for the colorimetric detection of some virus. The Ag@Fe3O4 nanoparticles are magnetic and plasmonic. They are arranged in monolayer array and 0-dimension on micro cover glass film. The film arranged with 175nm size particles is the most sensitive. When the virus is placed on film, we can see color changes with the naked-eye. In specificity test, first, we fix the antibody on the film. After that drop a droplet each virus sample of different concentrations onto the film. In sensing virus, the main reason why colors change is because of plasmonic coupling effect. This film sensor has a strong sensitivity that can be sensed up to the picogram unit. Thus, it shows high potential to become a new commercial virus diagnostic platform.

Poster Presentation : **ANAL.P-146**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of ultrathin Ni–Fe LDH nanosheets for efficient water oxidation

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In an electrochemical water splitting, developing a cost-effective, abundant and highly efficient electrocatalyst is a major challenge for the large-scale production of hydrogen and oxygen gasses. Recently, applications of transition-metal based layered double hydroxides as electrocatalyst in water splitting have attracted attention because of their abundance, stability and environmental friendliness. Here, an ultrathin nickel-iron layered double hydroxide (NiFe-LDH) nanosheet was synthesized through electrodeposition on to nickel foam (NF) substrates. In alkaline solution, the as-synthesized ultrathin nanosheet has exhibited an excellent oxygen evolution activity. Combined with its lower overpotential of 240mV at 10mAcm-2 and turnover frequency at overpotential of 400mV, and durability over 15, 000 s, this material is a promising electrocatalyst for water splitting.

Poster Presentation : **ANAL.P-147**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Evaluation of skin whitening efficacy of catechin by inhibiting mushroom tyrosinase activity

Young Jun Park

Food Science and Biotechnology, Cha university, Korea

Green tea, which is cultivated in island of Korean Jeju for a long time. It has been used mainly for dress to dye or drink. Main component of catechin has been known as anti-aging agent on the skin because of its excellent antioxidant effect. The purpose of this study is to present in vitro data on the activity inhibition of mushroom tyrosinase on skin as a measure of whitening efficacy. In addition, it will be observed that mushroom tyrosinase activity is inhibited depending on the concentration of the extract at 10, 100, 1000ppm. The activity inhibitory effect of mushroom tyrosinase will be expected meaningful difference on concentration. Finally, we will compare with the efficacy of well-known kojic acid of mulberry extract and conduct clinical demonstration on skin of animal/ human. Based on this research, we intend to develop a drug in the form of gel to lay the foundation for the pharmaceutical industry to treat skin lesion.

Poster Presentation : **ANAL.P-148**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

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

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Green tea has been cultivated in island of Korean Jeju for a long time. It has 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 for human. The proposal of this study will be determined whether the catechin compound mixture, the active ingredient, could be used as herbal extract to improve aging wrinkles, especially for middle aged group using various in vivo test. First, this study will determine its elastase activity and anti oxidant 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 compositon technology. It will add a step forward to the herbal pharmaceutical industry.

Poster Presentation : **ANAL.P-149**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of fluorine doped structured $Li_2FeP_2O_7$ and its electrochemical and structural characterizations

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Lithium-ion batteries (LIBs) as attractive power source have contributed to commercial success of electronic device. The LIBs have been predominately used in portable electronic devices, and its applications have expanded into electric vehicle (EV), energy storage system (ESS) and smart-grid technology. The motivation for using a LIBs relies on its high energy density, fast charge and discharge efficiency, stable operating at strict condition, and eco-reliability. As a cathode material, lithium metal pyrophosphates, $\mathrm{Li}M\mathrm{P_2O_7}$ (M = Mn, Co, Fe, V), have been subjected to intense recent research. Among them, $LiFeP_2O_7$ (LFPO) shows superior ionic diffusivity, inferior electronic conductivity and structural stability due to strong P–O bond as polyanion. Therefore, anion doping into the polyanion site can be able to improve intrinsic electrochemical properties such as band gap, and enhance lithium diffusion limitations. Consequently, fluorine anion (F^-) has been selected as a dopant in for oxygen sites. The fluorine doped LFPO has been synthesized by solid state reaction method. The structural study of the material has been investigated by X-ray diffraction and ^{7}Li MAS NMR. And the electrochemical performances have been characterized with designed galvanostatic cycling in various C rates and cyclic voltammetry (CV) measurement.

Poster Presentation : **ANAL.P-150**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

The targeted metabolomics profiling of urine in diabetic kidney disease using NMR

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Korea Basic Science Institute, Korea

Diabetic kidney disease (DKD) is a leading cause of end stage renal disease (ESRD), and the number of patients diagnosed with chronic kidney disease (CKD) and ESRD due to diabetes has been steadily increasing worldwide. To investigate the biomarker for CKD originated from DKD (DM-CKD), we performed the targeted metabolomics profiling using 800 MHz nuclear magnetic resonance spectroscopy (NMR). Prospectively urine samples consecutive patients with DM-CKD stage 1 to 5 (n=208) and controls (n=26) with normal kidney function were analyzed. We found a gradual elevation of glucose, mannose, fumarate, and pyroglutamate according to DM-CKD stages compared with control groups. These four urinary metabolites were significantly correlated with urinary protein-to-creatinine ratio and estimated glomerular filtration rate. After Kaplan-Meier analysis and multivariate Cox analysis, metabolites were associated with ESRD progression. This study demonstrates that the NMR based targeted-metabolomics shed light on understanding of the DM-CKD and enable us to predict the risk of ESRD progression.

Poster Presentation : **ANAL.P-151**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Quantitative multi-element analysis for assessing environmental exposure during early childhood with deciduous teeth

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Recently, deciduous teeth have received a great attention as new biomarkers for evaluating early-life human exposure due to their unique developmental process. Dentine layers of deciduous teeth are formed from the 14th to 19th week of pregnancy, so chemicals exposed during fetal period could be accumulated. In addition, exposure chemicals after birth are separated from prenatal exposure chemicals by a neonatal line which is formed at birth. These features make it possible for deciduous to have much longer tracking period than conventional biomarkers such as mother's blood, urine or placenta, cord blood. Our group has tried to develop a method for quantitatively measuring several elements from a baby tooth matrix. A developed method mainly consisted of a tooth matrix digestion by a microwave-aided acidic digestion and multi-element analysis by inductively coupled plasma dynamic reaction cell mass spectrometry (ICP DRC MS). Since deciduous teeth do not have a reference material, we used an NIST SRM 1486 bone meal, which is known to have the most similar components to those of tooth materials, for optimizing the analytical method. Our results showed that our method could successfully measure contents of over ten elements both from NIST SRM 1486 and from individual deciduous tooth samples.

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Poster Presentation : **ANAL.P-152**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Development and validation of a multi-element quantitation method for whole blood samples by ICP DRC MS

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In exposomics research that tries to measure all the exposures of an individual and reveal how the measured exposures relate to health, whole blood samples are one of the most widely used biomatrices due to its relatively easy accessibility and procedural simplicity. There have been many studies which tried to quantify elements from whole blood samples. Most of these studies focused on toxic heavy metals. For example, the US CDC laboratory manual published in 2014 described a method for quantitation of five toxic elements –cadmium, lead, manganese, mercury, and selenium- from whole blood samples. In this study, based on the US CDC laboratory manual, we tried to develop a multi-element analysis method with whole blood samples that can cover up to 12 elements including toxic heavy metals. In order to confirm the reliability of our method, we also performed validation of our method which include evaluation of detection limits, selectivity, precision, accuracy, and linearity.

Poster Presentation : **ANAL.P-153**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Antioxidative Activity of Oligosaccharides on UV-induced Photoaging in human skin cells

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Ultraviolet (UV) is one of the major reasons for the skin aging and its intracellular action mechanisms are well-defined as 1) mitochondrial damage due to UV-induced reactive oxygen species (ROS) and 2) collagen collapse in the subcutaneous layer due to increased expression of matrix metalloproteinase (MMP). Thus, antioxidants are commonly used as an anti-aging agents to inhibit free radicals produced by UV such as ROS. Oligosaccharides are kind of carbohydrates that have various biological activities such as improving intestinal environment and immune stimulation. Recently, antioxidant activity of oligosaccharides has been also identified from few kinds of oligosaccharides. In this study, seaweed-derived oligosaccharides were identified on anti-photoaging that was induced by ultraviolet B (UVB) irradiation in human keratinocytes (HaCaT cells). Reductive activity was validated using conventional ABTS assay with nine individual oligosaccharides and result indicated that neoagarooctaose (NA8) and neoagarodecaose (NA10) have reducing power. In HaCat cell-based antioxidant experiments, NA10 also inhibits ROS formation and ERK 1/2 phosphorylation. Finally, MMP-1 production was also interfered by NA10 treatment in HaCat cells. There experimental results suggested that NA10 has a potential for the skin anti-photoaging.

Poster Presentation : **ANAL.P-154**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Probing Structural Change of Protein using Small-angle X-ray Scattering (SAXS) and Cross-linking Mass Spectrometry

Chae Eun Heo, Chae Ri Park, MyungKook Son, Sooyeon Chae, Min Ji Kim, Paul Valery Migisha Ntwali, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Probing the protein-protein interactions are crucial for the study of wide variety biological system. Numerous research has been reported that various methods are developed to support the identification, characterization and analysis of protein complexes. Since the protein-protein interactions are influenced by PTM, metal ions, ion concentration has been reported that charged species abundant in our body (e.g. metal ion, DNA, nucleic acid, heparin, glycosaminoglycans etc.) influence to the mechanism of amyloid fibrillation by electrostatic interaction. Here, we have studied to understand the molecular mechanism of protein fibrillation under ATP, which is a small biological polyanion and is present in high levels in cell. Firstly, we have conducted the thioflavin T(ThT) assay which monitors the formation of amyloid fibril. To identify and characterize the protein complexes between protein and small molecules, we have utilized electrospray ionization mass spectrometry (ESI-MS) and ion mobility spectrometry (IMS), along with circular dichroism (CD) and solution small-angle x-ray scattering (SAXS). The experimental evidence obtained from these diverse analytical techniques, and subsequent studies about biological anion-mediated protein aggregation would be highly helpful in understanding the mechanistic details of amyloid fibrillation under the influence of external factors, which affect protein-protein interactions.

Poster Presentation : **ANAL.P-155**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

MS-based analysis of 2D and 3D spheroids neuroblastoma cells to explore mechanisms underlying cellular heterogeneity in neuroblastoma cell models.

Paul valery Migisha ntwali, Chae Eun Heo, MyungKook Son, Sooyeon Chae, Min Ji Kim, Chae Ri Park, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

MS-based proteomics of 3D cell model and single cell system has been extremely successful for quantitation of proteins that are integral components of essential processes for life and continues to revolutionize protein characterization. Development in different areas of proteomic workflow such as sample preparation, MS instrumentation and data processing have enabled us to get comprehensive information from MS-based proteomics. However, exploring cellular heterogeneity in tumors continues to be a challenge among researchers using cell models. Development of 3D cells has increased our understanding of cellular heterogeneity in tumor cells, an achievement which has caused the shift of recent researches towards the use of 3D cell culture. In this study, we optimized 3D spheroids cell culture condition by adjusting 3D scaffold and incubation conditions. Furthermore, we performed a comparative study of 2D and 3D spheroids cells by evaluating differences in anti-cancer drugs toxicity in these cell models. Additionally, ESI-MS was employed to highlight further differences between 2D and 3D neuroblastoma cells by emphasizing on differences in drug uptake mechanisms of these 2 cell models. This study will enhance our understanding of 2D and 3D spheroid cell model impacts in optimizing the efficacy of anti-cancer drugs and will contribute to the development of pre-treatment methods of 2D and 3D spheroid model for MS-based proteomics.

Poster Presentation : **ANAL.P-156**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Characterization of Structural Change of Protein during Gas Phase Transition Using Electrospray Ionization (ESI) with Fourier Transform-Infra red (FT-IR) spectrometer

MyungKook Son, Tae-Won Ko, Chae Eun Heo, Chae Ri Park, Paul Valery Migisha Ntwali, Sooyeon Chae, Min Ji Kim, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Electrospray ionization (ESI), is a soft ionization technique that produce gas phase ions by applying high voltage to a sample solution. Solution samples are sprayed into air, creating gas-phase ions by evaporation process. ESI coupled with ion mobility mass spectrometry (IM-MS) has been widely used to study gas-phase ions, which produces information of gas-phase structures of the ions. Many researchers have been utilized ESI-IM-MS to study solution phase structure of proteins by relating with gas-phase structures. However, there is no evidence whether the conformations of proteins are intactly preserved during the evaporation process.. So, to observe the phase transition of protein ions from solution to gas phase, we built home built ESI coupled with Fourier transform-infra red (FT-IR) spectrometer. We firstly monitored lysozyme in deuterium oxide-tris buffer to see IR spectrum of the alpha helix peak of protein. Hopefully, the results of this study will help to elucidate how gas-phase protein ion conformations are formed, or if the gas-phase conformation is directly related to the solution-phase conformation of proteins.

Poster Presentation : **ANAL.P-157**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Inhibition and dissociation effect of gold nanoparticles on amyloid fibrils induced by Near-IR laser irradiation

Chae ri Park, Chae Eun Heo, MyungKook Son, Min Ji Kim, Sooyeon Chae, Paul Valery Migisha Ntwali, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Amyloid-β (Aβ) fibrils, which are self-assembled peptides of Aβ, have been regarded as pathogenic hallmarks in Alzheimer’s disease. To remove the amyloid fibrils, several studies have been tried to dissociate fibrils by physical stimulation such as NIR radiation nanoparticles. In these regards, some metal nanoparticles have been reported not only to inhibit amyloid fibril formation but also dissociate preformed fibrils with a photothermal effect under NIR light. However, it has not yet been revealed how fibril dissociation is affected by the size, shape, and ligand of nanoparticles and NIR laser power. Here, we have studied dissociation characteristic of amyloid fibril using star-shaped gold nanoparticles under NIR laser irradiation. First, we synthesized star-shaped gold nanoparticle with the size of 60nm. Then, after applying 1W 808nm NIR laser for several minutes, we found amyloid fibrils are partially disintegrated with these gold nanostars. In this process, we used thioflavin T (ThT) assay to monitor the formation of amyloid fibrils and identify the changed quantity of fibrils after laser irradiation. To identify the morphology and structural characteristics of amyloid fibrils, we used a transmission electron microscope (TEM), circular dichroism (CD), FT-IR spectrophotometer, etc. The results obtained from these analytical techniques will help us to search ideal characteristics of size and shape, ligands of nanoparticles, which act as a disrupter of amyloid fibrils.

Poster Presentation : **ANAL.P-158**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Comparison of Solvent Effects on Cytotoxicity of Pt-based Drugs in 2D Cells and 3D Spheroid Cells

Min Ji Kim, Chae Eun Heo, Sooyeon Chae, Paul Valery Migisha Ntwali, Chae Ri Park, MyungKook Son, Da Gyeong Hyun, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Cisplatin (cis-[Pt(NH3)2Cl2]), a first-generation metal-based anticancer drug, has been widely used to treat diverse cancers including pediatric cancers. Cisplatin is commonly administered as a single drug or in combination with other drugs to raise its efficacy. Nevertheless, cancer cells could have acquired or intrinsic resistance to cisplatin. For this reason, a large number of in vitro studies have been conducted to clarify the mechanism of this phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin and other drugs due to its ability to dissolve drugs in high concentration. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl-. To understand how DMSO directly impede platinum (Pt)-mediated toxicity, we employed 3 dimensional spheroids and 2 dimensional monolayer of SK-N-SH neuroblastoma cells to understand cisplatin activity in the presence of DMSO. Then we employed an inductively coupled plasma mass spectrometry (ICP-MS) for the quantitative analysis of cisplatin. Our quantitative results show that cellular uptake and DNA-Pt adduct formation is significantly reduced for the cells treated with cisplatin dissolved in DMSO compared to those treated with cisplatin dissolved in media. Overall, our study would provide valuable insight into the reduced efficacy of cisplatin for cancer treatment in the presence of DMSO, based on the correlation with structural change of cisplatin induced by DMSO.

Poster Presentation : **ANAL.P-159**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Uncovering dose-dependent chemoresistance of serum-starved SK-N-SH neuroblastoma cells against the anticancer drug

Sooyeon Chae, Min Ji Kim, Paul Valery Migisha Ntwali, Chae Eun Heo, Chae Ri Park, MyungKook Son, Hugh I. Kim*

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Neuroblastoma is a solid tumor that arises from the sympathetic nervous system with complex, heterogeneous clinical behaviors. Chemotherapy is widely used to treat neuroblastoma and many studies have attempted to decipher the action mechanism of anticancer drugs. however, in spite of complex, heterogeneous of neuroblastoma, chemotherapy regimen is fixed and not consider heterogeneity of tumor cells. In this study, we investigated the effects of different concentration of topotecan on human neuroblastoma SK-N-SH cells under varying nutrient supply conditions. The survival rate of serum-starved SK-N-SH cells increased upon treatment with a high concentration (1 μM) of topotecan. Using quantitative proteomics and network analysis, we showed that topotecan (1 μM) upregulated DNA repair and cholesterol-mediated topotecan efflux, resulting in topotecan resistance. Time-resolved topotecan quantitation using multiple reaction monitoring mass spectrometry further supports that topotecan resistance was associated with enhanced drug efflux. Our results provide a model for high-dose-dependent chemoresistance in neuroblastoma cells that could enable a patient-dependent chemotherapy screening strategy.

Poster Presentation : **ANAL.P-160**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Biodegradation Evaluation of Biodegradable Microcapsules for Medical and Industrial Applications

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Microcapsules are materials used in various fields such as medicine, cosmetics, and fabric softeners, and microcapsules are often synthesized into microplastics in household goods. However, as plastics are the main culprit of ecosystem destruction and environmental pollution, many countries are declaring war on plastics around the world. Therefore, we attempt to synthesize biodegradable microcapsules and check their biodegradation in various ways. We selected biodegradable polymers through theoretical investigations and synthesized cellulose-based microcapsules using biodegradation studies of NMR-based cellulose using enzymes. Synthesis of microcapsules was confirmed by microscopy, IR and NMR, and residual isocyanates that may remain during microcapsule synthesis were analyzed by IR and NMR to check for harmlessness to the human body. To confirm the biodegradability of the synthesized microcapsules, we performed BOD, COD and cellulase-based degradation experiments.The enzymic study was measured by NMR, UV spectrum, and SEM, and the change over time was confirmed. The biodegradation of microcapsules could be predicted through the change of line width, absorbance, and morphology. The biodegradability tendency of the samples shown by each experiment did not deviate significantly from the expectations based on the raw material used for the synthesis. Currently, we are conducting more various control experiments, focusing on experiments to verify whether the changes caused by cellulase are correct, and trying to develop biodegradation confirmation methods applicable to microcapsules that will be useful in medicine and industry.

Poster Presentation : **ANAL.P-161**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Hybrid Magnetic Carbon Nanoparticles for Removal Organic Dyes

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The elimination of organic dyes from the wastewater of textile and food industry companies is a serious environmental issue. Nowadays, there are numerous materials are used for organic contaminants treatment, however, they are difficult to reuse and separate. Herein, we show the fabrication of hybrid magnetic carbon nanoparticles (MCNs) with different shapes for removal the organic dyes because of facile separation and reusability. Three different shapes are multi-shell, core-shell and cross-linker and they were synthesized by polydopamine and iron precursor. The MCNs morphology, structure and surface area were confirmed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and Brunauer-Emmett-Teller (BET). Moreover, the three systems were investigated the removal efficiency. The cross-linker shape was shown the highest efficiency for adsorption the organic contaminants because of high surface area. Furthermore, the commercial activated carbon (M200) was linked with magnetic for comparing the efficiency with the cross-linker MCNs. Hence, these MCNs can perform as an excellent adsorbent with various benefits of reusability and facile separation.

Poster Presentation : **ANAL.P-162**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

New analytic method to measure the atomic weight of neon using GC-TCD

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The atomic weights of neon gases have been measured by means of gas chromatography with thermal conductivity detector (GC-TCD). We have employed the high purity neon (Ne) gases as the carrier and sample gases in this study, and this is differentiated with typical GC analysis. The peak signals from the gas chromatography with thermal conductivity detector (GC-TCD) appear when the thermal conductivity between the sample and carrier gases is inconsistent. In most gaseous molecules, the thermal conductivity is consistent with the same chemical species. However, the thermal conductivity of Ne gas shows the discrepancy among several manufacturers, since the relative abundance of ^{22}Ne isotope is a quite large by ~10 % in atmospheric Ne and varies due to the mass fractionation during an air separation.We have identified the atomic weights of six Ne gases, which were used as three samples, and three references. The atomic weights of three Ne samples and one carrier gas were unidentified in the past, and in case of other three Ne references, the absolute isotope ratios were previously reported. We have performed the linear regression using GC peak areas of three references to determine the atomic weights of Ne samples. The atomic weights of three Ne samples results from linear regression were 20.1789 (2), 20.1802 (2) and 20.1828 (2) g mol^{-1}, respectively.To verify the atomic weights results from GC-TCD measurements, the absolute isotopic ratios of all Ne gases were measured by using the magnetic section-type gas/mass spectrometer. The atomic weights of the seven Ne gases, including the carrier gas, were compared with those results from GC-TCD and the GC-TCD results were well agreement within the expanded uncertainty (k = 2).

Poster Presentation : **ANAL.P-163**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

lipidomic analysis of serum from mice exposed to ambient particulate matter using LC-MS approach

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Ambient particulate matter(PM) has known as environmental risk factors in Korea, and associated with disease including asthma, cardiovascular and nervous disorder. However, the molecular mechanism by exposure to PM has not been fully understood.. We observe the metabolic perturbations in response to PM with a diameter 2.5-10 µm (PM10) exposure in mouse model. In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3 weeks in chambers. We conducted untargeted lipidomic analysis of serum from mice to evaluate metabolic perturbations using ultra performance liquid chromatography/quadrupole time of flight mass spectrometry (UPLC/Q TOF MS). Partial least squares - discriminant analysis (PLS-DA) score plots showed a clear separation between the PM10 exposed group and control group. We observed changes in lipids including ceramide, free fatty acid, acylcarnitine, phospholipid and diacylglycerol species in PM10 exposed mice compared to control. phospholipid species were decreased in PM10 exposed group compared to control, whereasacylcarnitine and free fatty acid species were significantly increased in PM10 exposed group, indicating the alteration in fatty acid oxidation metabolism. This study demonstrates that the LC-MS based-lipid profiling can be a used to understand the metabolism of PM10 exposed group on biological system.

Poster Presentation : **ANAL.P-164**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Characterization of Various Refined Lacquer Saps with Analytical Techniques

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Traditionally in Asian countries, lacquer sap was used as surface coating materials to protect, decorate and paste various materials such as wood, ceramic, paper and leather. The commonly used lacquer sap which is extracted from three main lacquer trees has mixtures of various catechol or phenol substitutes with C15 and C17 side chains such as urushiol, laccol and thitsiol. Lacquer was used in Korea for a long time and the research was needed to inherit the traditional heritage and to develop the usage by standardization and advancement. In this study, the chemical and physical properties of the raw lacquer saps were obtained from different countries: Korea, China, and Vietnam. And also refined lacquer sap by various refining time was investigated. The refinement was done by vaporizing water at room temperature and made to be homogeneous. The properties of refined lacquer was studied by purifying time period to investigate the change of components and physical properties. The lacquer films to determinate the physical characteristics were coated approximately 10 μm thick on 4 different materials: Si wafer, glass, acrylic panel and stainless steel plate, and were stored at 25 °C with 75% humidity. Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), High Performance Liquid Chromatography (HPLC), and Pyrolysis-Gas Chromatography-Mass Spectrometry (Py-GC/MS) were used to provide the structural information and contents of a series of catechol derivatives of three different countries lacquer. In addition, various analysis techniques were performed to measure the adhesion energy and hardness using peel tester, pencil hardness tester, Atomic Force Microscope (AFM) and Nano indenter.

Poster Presentation : **ANAL.P-165**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Average structure parameters of Asphaltenes by Magnetic resonance spectroscopy

Yongnam Joe

Analysis unit, Sk Innovation, Korea

Petroleum derived asphaltenes are known to be the most complex fraction of crude oil. They are also known to be coke precursors in refinery process resulting in several problems such as catalyst deactivation and poisoning because of their tendency to flocculate and precipitate during oil upgrading process. It is neeed to understand more thoroughly the structures and behaviors of asphaltenes to predict their chemistry during refining process. However, petroleum asphaltenes are very complex aromatic molecules surrounded and linked by aliphatic chains. The inherent complexity of asphaltenes hinders a full identification of their constituents. A great variety of analytical techniques including various types of chromatographic methods and spectroscopic methods have been employed to investigate asphaltene molecular structure and still many things are going on. Among them NMR is a powerful analytical method as it allows to quantify different types of protons and carbons. Average structure parameters such as aromaticity, degree of ring condensation and alkyl chain length can be evaluated by means of NMR.Also, asphaltenes contain unpaired electrons and form complexes with vanadium. By EPR analysis organic asphaltene radical and vanadyl porphyrin can be discriminated. EPR can detect these species in order to determine the asphaltene content and can be used to understand the characteristics of asphaltenes. It can be used to predict reactivity of refinery process such as hydrotreating demetalization process.In this work, we present the magnetic resonance spectroscopic work such as Liquid-NMR, Solid-NMR and EPR on petroleum derived asphaltenes in order to evaluate the structural aspects that could be correlated with crude oil behavior in thermal process.

Poster Presentation : **ANAL.P-166**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Multiple omics analysis related to mesenchymal stem cell mass cultivation

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Biotechnology products and medicines based on stem cells are being developed in variety. The development of stem cell bioproducts and therapies require a large amount of stem cells. In order to develop such products, it is necessary to process a culture system capable of mass production of stem cells. We carried out experiments with the aim of developing technology to monitor stem cell culture markers through quantitative analysis of metabolites and proteins related to cell growth and proliferation. “Additive A” was inserted into the control media to develop a medium in which the proliferation rate of stem cells was fast and the morphology of the cells were not altered. The mesenchymal stem cells were cultured for 5 time points (6 hours, 1 day, 2 days, 3 days, and 4 days) in the new media which is added Additive A and the control media. As a result, it was found that glutamine and sugar were consumed more in the new media than in the control media, and this shows that the cells of the new media required more energy which is needed for cell proliferation. Proteome quantification was performed by clustering the ratio of the control media to the new media according to the time points. As a result, we observed biological processes and KEGG pathways related to Additive A in the cluster which show a decreasing pattern over time. We conclude that Additive A is involved or helps in cell proliferation.

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Poster Presentation : **ANAL.P-167**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Utilizing accurate precursor mass information from MS data for interpreting data-independent acquisition(DIA) mass spectrometry significantly improves peptide identification

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Data-independent acquisition (DIA) has emerged as a promising strategy largely owing to developments in advanced mass spectrometers and sophisticated data analysis methods. However, DIA produces highly complex multiplexed tandem MS spectra which makes it difficult to interpret. Here, we present a novel strategy to analyze DIA data, based on unambiguous precursor mass assignment through the mPE-MMR (multiplexed post-experimental monoisotopic mass refinement) procedure, and combined with complementary multi-stage database searching. Compared to conventional spectral library searching, the accuracy and sensitivity of peptide identification were significantly increased by incorporating precise precursor masses in DIA data. We demonstrate identification of additional peptides ab-sent from spectral libraries, including sample-specific mutated peptides and post-translationally-modified peptides using MS-GF+ and MODa/MODi multi-stage database searching. This novel strategy shows considerable potential for interpreting DIA data and further exploited by adopting methods that support to obtain high-dynamic range of MS data.

Poster Presentation : **ANAL.P-168**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Efficient and comprehensive proteomic analysis by fully automated DO-NCFC-RP/RPLC

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Recently, human proteome analysis from a single-cell type covering 10,000 proteins is practicable, although some methodological and technical issues remain. There are still significant challenges to identify more than 10,000 proteins, because the identification efficiency of present technology has decreased at this level of identification. Here, we report a dual online reverse-phase/reverse-phase liquid chromatography system, which utilizes an online non-contiguous fractionating and concatenating device (NCFC fractionator). In shotgun proteomics analyses of a human proteome, this system provides considerably improved exploitation of the separation space, resulting in a significant increase in the numbers of proteins identified compared to a general contiguous 2D-RP/RPLC method. Unlike the previously described offline 2D-NCFC-RP/RPLC method, the completely automated online 2D-NCFC-RP/RPLC system bypasses complex manual processes such as offline fractionations, pooling, clean-up, drying, reconstitution, and autosampler fraction injection. As a result, our novel system offers minimal sample loss and highly reproducible 2D-RP/RPLC experiments. With this system, in single shot data-dependent acquisition (DDA), we identified more than 10,000 proteins in one-day data acquisition time. In addition, we performed data independent acquisition (DIA) experiment, which has emerged as an alternative approach to data dependent acquisition (DDA) for comprehensive proteomic analyses. We will discuss the comparison of DIA and DDA data.

Poster Presentation : **ANAL.P-169**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Investigation of Physical Properties in Nano-structured Copolymer Films by Atomic Force Microscopy

Minhwa Kang, Jihye Lee, Yeon Hee Lee*

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Microphase separation is normally observed in block copolymer films when the equilibrium of a polymer film is broken by external circumstances such as pressure or temperature. Block copolymer film is consist of two or more homopolymers linked with covalent bond. As the annealing condition is controlled, the morphology of block copolymer film is changed to ordered arrangement. The block copolymer films have various nano structure like cubic, hexagonal, bicontinuous and lamellar depending on the volume fraction of each homopolymer. In this study, Atomic Force Microscopy (AFM) was used to obtain the information of nano-structured diblock copolymers and blend homopolymers. The AFM results from various modes provided the information about the surface morphology, physical properties and microphase separated structure of the copolymer films before and after annealing treatment.

Poster Presentation : **ANAL.P-170**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Construction of substrate PI property analysis process applied to flexible OLED.

Ji Sun Kim

Chemical analysis technology team, LG Display, Korea

Recently, as the need for 'flexible displays' using light and flexible plastic substrates instead of conventional glass-based displays is increasing, competition in R&D and industrial production by country and enterprise is fierce. In addition, OLED made of organic materials that emit light without backlight have been actively developed as flexible displays due to excellent flexibility. These flexible displays are wholly dependent on the substrate and in the case of transmissive displays, not only flexibility but also optical clarity are important factors. In order to develop a substrate, it is important to understand the required properties of the plastic substrate used and to select a polymer materials. Development of transparent plastic substrates for flexible displays has been in progress since the late 1990s, and nowadays, polyimide (PI), which can show the thermal characteristics of glass level, is commercially used as the sole substrate of the flexible display. PI has the advantages of superior elasticity, impact resistance and light transmittance and it has chemical resistance, abrasion resistance, and heat resistance and stability to external stimulation. In addition to the above, there are advantages such as excellent mechanical and electrical properties.The purpose of this study is to evaluate the properties of PI films to derive material management items, to secure material stability through periodic monitoring, and to analyze the correlation among material companies. To assess the overall properties of PI, various analytical techniques were used. As a result, we will support the evaluation of the mass production process, manage the items to identify and improve the cause of defects, and establish a comprehensive PI substrate analysis process.

Poster Presentation : **ANAL.P-171**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Structural and mechanical properties of jewel beetle elytra

Jihye Lee, Yeon Hee Lee[*]

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

The elytra of jewel beetle, which are metallic green with red stripes, have been used as an ornament from ancient times because of their colorful colors, light mass and high strength. In particular, the elytra of jewel beetle have more than 15 layered structures, making them easy to reflect a lot of light, so they have a structural coloration that looks different in color depending on the angle of view. Investigation of this ingenious structure is very interesting topic not only for the arts and cultural heritage conservation, but also for the researchers who want to apply it to biomimicry. In this study, surface analytical instruments such as AFM and nano-indenter were used to investigate structural and mechanical properties of elytra. The surface morphology and phase, lateral force, and surface potential were measured by AFM. The cross sectioned samples of two different color areas (green and red) by FIB and also measured by AFM. And the hardness and thickness of the multilayer were verified with nano-indenter.

Poster Presentation : **ANAL.P-172**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Extensive proteome profiling of IDH1 mutated U87MG cell line for investigating the tumorigenic roles in glioblastoma

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Glioblastoma is the lethal type of brain cancer. A recent genomewide mutational analysis of glioblastoma revealed IDH1 mutation was associated with an increase in overall survival in patients. However, proteome research related with the IDH1 mutation have not been systematically reported. Here, we present comprehensive proteomic analysis of IDH1 R132H point mutated U87MG cell line for investigating the tumorigenic roles in glioblastoma.For deep proteome profiling, 6-plex TMT labeling was performed on day 1 and day 6 samples: each of wild type, mutant 9-6 and mutant 9-19 cell line respectively. For phospho analysis, IMAC enrichment was performed on pooled 2.4 mg peptide samples and the flow-through was divided into 24 fractions using mid-pH RPLC fractionation. Phosphopeptide analysis was performed on Q Exactive HF-X which was coupled to a DO-2D-NCFC-RP/RPLC system and 24 fractionated global peptide samples were analyzed by Q Exactive HF-X which was coupled to a DO-RPLC system.An extensive profiling generated comprehensive proteome information including avg. 259,060 peptides, 11,868 protein groups and avg. 51,595 phosphopeptide. 7,352 protein groups for global and phospho analysis respectively.

Poster Presentation : **ANAL.P-173**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Comprehensive proteome profiling to investigate RNAlater effect on the human Pancreatic ductal adenocarcinoma (PDAC) tissues

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Proteogenomic study of PDAC is particularly challenging because the tissues contain a variety of enzymes including DNases, RNases and proteases that can lead to degradation of RNA and proteins. For this reason, RNAlater is often used to protect RNAs of PDAC tissues. High concentration of quaternary ammonium sulfates of RNAlater is known to protect RNA from degradation for long time storage. However, it is still unknown whether RNAlater affects the qualitative and quantitative information of proteome and phosphoproteome.In this study, we carried out comprehensive global proteome and phosphoproteome analysis to investigate the RNAlater effect on the PDAC tissue. Tissues from three patients were individually pulverized and the tissue powders of each patient were divided into two groups. One group was kept in RNAlater at 4°C and the other group was stored at −80°C both for 24 hours. Tissue powders were digested using FASP method then labeled with 6-plex TMT. Labeled samples were separated into 24 fractions by mid pH RPLC. A portion (~8%) of each mRP fraction was subjected to LC-MS/MS to profile the global proteome and the remaining samples (~92%) were concatenated into 12 fractions, which were each performed IMAC phosphopeptide enrichment. As a result, the global proteomic profiling identified 99,163 unmodified peptides of 8,803 protein groups, and phosphoproteomic analysis resulted in the identification 17,345 phosphopeptides of 16,436 phosphosites.Our data showed that RNAlater has negligible effects on both global proteome and phosphoproteome of PDAC tissue. Thereby the use of RNAlater to protect both RNAs and proteins of PDAC tissues is a viable method for proteogenomic studies on PDAC.

Poster Presentation : **ANAL.P-174**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Monitoring the changes of mitochondrial membrane potential using SERS in the live single cell

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Obtaining the molecular information from inside cell in real time has been a critical issue to study the interaction between molecules of interest and intracellular components. Fluorescence-based technique has been an excellent tool to study such important interactions for years. We are demonstrating the Raman scattering based method as a promising platform to achieve the real-time monitoring of the subtle molecular changes occurred in inside cells. The triphenylphosphine-modified AuNPs were selectively localized in the mitochondria and showed the characteristic Raman spectrum of cytochrome C and other Raman spectrum of molecular components inside cell. The Raman scattering based method enabled to observe the changes of mitochondrial membrane potential in the single cell of rheumatoid arthritis synovial fibroblasts induced by protein (TNF-a), various chemicals ($MgCl_2$, sodium pyruvate, FCCP), and non-chemical stimulus (i.e., light). The surface-enhanced Raman spectrum originated from mitochondria were sensitively changed with time when induced mitochondrial depolarization by the additions of TNF-a, or chemicals to induce the changes of mitochondrial membrane potential.

Poster Presentation : **ANAL.P-175**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Lipidomic analysis of elaiosomes from Coreanomecon hylomeconoides Nakai by high performance liquid chromatography- tandem mass spectrometry

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

Elaiosome is a small structure attached to a seed and mainly consists of lipids. The main role of elaiosome is to attract ants to disperse the seeds of plants from place to place. High performance liquid chromatography-electrospray ionization-tandem mass spectrometry (HPLC-ESI-MS/MS) was used to profile and quantify the lipid contents in the elaiosomes of Coreanomecon hylomeconides Nakai, which is endemic species in Korea. Lipids extracted from elaiosomes sampled in seven different populations were subjected to relative quantification using a quadrupole-time-of-flight mass spectrometer in both positive and negative ion modes. More than 85 lipid species including glycerophospholipids and triglycerides were identified in each of pooled samples analyzed in triplicate. The majority of fatty acyl chain composition of the identified lipids were C16:0, C16:1, C18:1, and C18:2, These results were consistent with the previous studies on the composition of elaiosome free fatty acids, which are regarded as key players in the mutualistic relationship between and ants. Finally, statistical analyses were conducted with the R software to differentiate lipidome among the seven populations.

Poster Presentation : **ANAL.P-176**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Quantitative lipidome analysis of serum from mouse exposed to microplastic using deuterium oxide labeling

Jin Young Park, Tae-Young Kim*

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

Microplastics are small (typically less than 5 mm) pieces of plastic fragments and have become global environmental and health concerns due to pollution of the aquatic system including oceans, rivers, and lakes as well as air and soil. Most studies on the health risks caused by microplastic exposure have been conducted on marine organisms with high concentrations of microplastics. To study the in vivo effects of low concentrations of microplastics on mammal, untargeted lipidomic analysis was performed with a mouse model based on Deuterium Oxide (D_2O) Labeling for Global Omics Relative Quantification (DOLGOReQ) technique that we have recently developed. For experimental group, ICR mice were administrated with microplastics in drinking water for 5 weeks. The plastic concentration was set to consume 386.82 ng of polyethylene (PE) and polystyrene (PS) per day. Four and five replicates of mice were exposed to PS and PE, respectively. The concentration of plastic in drinking water was changed weekly based on the mouse weight. For the control groups, four replicates of ICR mouse were fed by either normal drinking water or 5% D_2O enriched drinking water. After 5 weeks, serum samples were collected from both experimental and control groups. Lipids were extracted from mouse serum using Folch method. Lipid extracts were analyzed by high-performance liquid chromatography-mass spectrometry. Finally, relative quantification of lipidome between experimental and control groups was performed by DOLGOReQ. A total of 212, 176, and 301 lipids were identified from control, PE, and PS groups, respectively. Among them, 136 lipids were commonly identified. In the relative quantitative analyses, 2 sphingomyelins in PE exposed group and 2 glycerophosphoethanolamines in PS exposed group showed significant changes compared with control group.

Poster Presentation : **ANAL.P-177**
Analytical Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Digital rectilinear ion trap mass spectrometer

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Department of Chemistry, Sogang University, Afghanistan

We present the demonstration of digital rectilinear ion trap (RIT) mass spectrometer. We designed and manufactured the RIT based on the design of Ouyang et al. For the operation of this mass analyzer, we applied concepts of the digital ion trap, in which RF voltages of the rectangular waveform was applied to the electrode, not typical sign waveform. Besides, the mass scan is also done by frequency scan, not by voltage scan. In this research, we used the FPGA controller for the generation and control of the rectangular waveform. Circuits composed of two high power/RF MOSFETs were also made to generate trapping voltages. All I/O communication was controlled by home-built LabVIEW software. We plan to conduct the performance experiment of this mass spectrometry in detail and expand it for more sophisticated analyses.

Poster Presentation : **ANAL.P-178**

Analytical Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Development of an automatic sample preparation system using a Lab-on-a-Disc

Hwa-yong Jang, Han Bin Oh*

Department of Chemistry, Sogang University, Afghanistan

A disc for the lab-on-a-disc analysis was designed and constructed to automatically perform sample preparation for quantitative analysis of formaldehyde using LC-MS/MS. This disc was designed to perform a series of well-organized sample preparation steps, such as mixing and filtering, automatically on the lab-on-a-disc. In addition, an instrument that can perform the lab-on-a-disc analysis was also made in-house, which utilized the feedback loop of several serial communications between an arduino microcontroller and a LattePanda microcomputer board to control the fluid movement and precisely measure a number of real-time revolutions. Further, a high-speed image capturing system was also implemented to monitor fluid movements.

Poster Presentation : **LIFE.P-179**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Bioactive MOFs embedded Hydrogels

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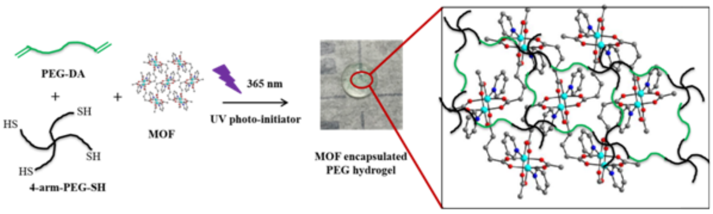
Three metal-organic frameworks (MOFs), Cu-MOF **1**, Co-MOF **2**, and Zn-MOF **3** containing glutarate and 1,2-bis(4-pyridyl)ethylene ligands were synthesized by hydrothermal or solvothermal reaction. Bioactive MOFs embedded hydrogels, hydrogel@MOFs **4-6** were prepared by UV light mediated thiol-ene photo-polymerization using diacrylated PEG (PEG-DA), 4-arm thiolated PEG (4-arm PEG-SH) and MOFs. The antibacterial activities of three hydrogel@MOFs **4-6** were tested against Gram-positive and Gram-negative bacteria. Although these hydrogel@MOFs are confirmed to be very stable from releasing M^{II} ion test of hydrogel@MOFs in the medium utilized for antibacterial tests, two hydrogel@MOFs **4 and 5** showed very excellent antibacterial activities against two bacteria. The robust porous frameworks rather than released M^{II} ions from hydrogel@MOF participate more strongly in inactivating bacteria and reducing cytotoxicity caused by free metal ion. The central metal was supposed more important factor to affect on the bacteria than chemical properties of ligands.



Scheme. Schematic representation of UV-light-activated bioactive MOFs-embedded PEG-based hydrogel formation.

Poster Presentation : **LIFE.P-180**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Mimicry of the Cytoskeleton: Actin and Microtubule Polymerization in Giant Unilamellar Vesicle causing Shape Changing

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Microtubule and actin cytoskeletons are physically contacted in a cell and dynamically coordinated to play vital roles in many cell functions, from migration, growth, and division. These structural dynamics of cytoskeletal proteins are of interest, the physical roles of cross-linking proteins between two filaments have been identified. Yet most studies were performed in a highly controlled interface or a bulk. Recently, we developed to simulate a cytoskeleton formation through ATP-dependent actin polymerization in a giant unilamellar vesicle (GUV) Optical stimulation-initiated ATP synthesis and induced ATP-dependent actin polymerization, leading to the growth of three-dimensional highly curled actin filament network. In this study, we further added the ingredients for microtubule formation into the actin polymerizable GUV system and controlled both of the polymerization via single divalent cation Mg2+. Also, by adapting the lipid phase separation techniques in the GUV system, the GUV could bare any physical forces generated during the polymerizations. We will discuss how the lipid phase-separated GUV showed structurally and shape change during the cytoskeleton proteins polymerization. At last, we will discuss how these shape changes and the cytoskeleton co-polymerizable GUV system could lead to artificial cellular movements in future research.

Poster Presentation : **LIFE.P-181**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Fibronectin coated Polydioxanone Surgical Suture for Wound Healing Improvement

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Polydioxanone (PDO) is one of polymer for suture material of abdominal and aesthetic plastic surgery procedure; to hold tissues until the healing process is complete. Although it is biodegradable and biocompatible, secondary infection, delayed wound healing and scar formation are the most frequent complications after surgical interventions. Therefore, novel technology is required to prevent these shortcomings. Fibronectin, the most prominently extracellular matrix component, has domains to bind integrin receptor to enhance adhesion-dependent cell growth. Here, the surface of PDO suture is modified to attach fibronectin. The result showed that after surface modification, fibronectin adsorped and attracted fibroblast, the key player of wound healing, on PDO surface. Fibronectin coated PDO sutures significantly enclose the wound compared to the control group in an in vitro wound-healing assay. This can be confirmed by increasing released fibronectin from the sutures to physiological like a buffer. This study presents an innovative approach to use surgical suture as fibronectin delivery for regenerative features and improve the tool to promote wound healing after a surgery procedure.Keywords: polydioxanone, surgical suture, fibronectin

Poster Presentation : **LIFE.P-182**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Sensitive Detection of CCP peptide Using Metal-Enhanced Fluorescence Nanoparticles

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Rheumatoid arthritis (RA) is a chronic autoimmune disease which causes severe damage to the joints and leads to serious mobility impairment. Because there are many complications of RA, it is important to make a correct diagnosis and start treatment before significant joint damage progress. One of the most useful biomarker for early diagnostics of RA is anti-cyclic citrullinated peptide antibodies (anti-CCP). These are considered highly specific for RA in comparison with Rheumatoid Factor (RF), so that the required test systems have been continuously optimised in the past years.Currently, enzyme-linked immunosorbent assay (ELISA) is a conventional method for anti-CCP detection. Although ELISA is a convenient technology, low limit of detection (~25 U/mL) and high background noise remain problems. Therefore, we will improve the sensitivity using metal-enhanced fluorescence nanoparticles and microarray on Dendron modified surface.In this work, we suggest new approaches to supersensitive analysis of anti-CCP using metal-enhanced fluorescence (MEF) nanoparticles and microarray. To detect anti-CCP, we immobilized CCP peptide on Dendron coated glass slide and use fluorescence labeled anti-human antibody. This approach is expected to be a useful tool for early RA diagnosis that can detect low concentration of anti-CCP.

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Poster Presentation : **LIFE.P-183**
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Quantitative Analysis of LIMK1 in a Single Cell with Atomic Force Microscopy

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Proteins are essential parts of organisms and participate in virtually every process within cells, performing a variety of functions. LIM domain kinase 1 (LIMK1) is a multifunctional protein and is involved in regulation of cell motility, cell cycle, cytokinesis and cellular morphology. LIMK1 also regulates neurite growth, synaptic stability, growth cone motility, axon formation through modulation of Golgi dynamics and neuronal differentiation. This protein stimulates axon growth and may play a role in brain development. In particular, LIMK1 hemizygosity is implicated in the impaired visuospatial constructive cognition of Williams syndrome, which is a unique neurodevelopmental disorder characterized by severe defects in visuospatial cognition and long-term memory. Accordingly, quantitative analysis of LIMK1 and their distribution in a single cell is important to study the biological role of LIMK1 in neurons.Conventional methods for protein analysis including western blotting, ELISA, and immunofluorescence have some problems that they have low detection limit and use fluorescent molecules. Therefore, atomic force microscopy (AFM) is a good candidate to overcome the hurdles. Using the mapping capability of AFM, it is possible to obtain a map the distribution of a specific protein in a naonometric resolution without modification or amplification. In this way, LIMK1 can be analyzed quantitatively in a single cell and their distribution can be mapped at high lateral resolution.

Poster Presentation : **LIFE.P-184**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Multifunctional Glycosylated Fluorescent Probes for Assessment, Imaging, and Separation of Glycosidases

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Glycans are biopolymers containing oligosaccharides and polysaccharides, and are usually observed in the form of glycoconjugates such as glycoproteins, proteoglycans, or glycolipids. Contrary to other biopolymers that are synthesized in a template-dependent manner, glycans are produced step by step by glycosyltransferases and glycosidases without any template. Moreover, glycans affect the activities of biopolymers to which they are combined by controlling their functions.Glycosidases, which catalyze the cleavage of glycosidic bonds in glycoconjugates or other various biopolymers, play key roles in carbohydrate metabolism of living organisms. Therefore, it is highly required for research on carbohydrates to study functions of glycosidases furthermore.Here, a multifunctional near-infrared glycosidase probe is newly suggested. Near-infrared (NIR) dyes were synthesized instead of conventional UV-Visible dyes since most of the background signals such as autofluorescence from biomolecules are in the UV-Visible region. That is, unnecessary background signals are minimized in the near-infrared region. Various substrates such as D-galactose or N-acetyl-D-glucosamine were attached to the optically tunable position of NIR dyes via a glycosidic bond so that cellular glycosidases selectively cleave the glycosidic bonds and form enzyme-probe complexes. By this, the target enzymes are labeled and their activities are characterized by NIR fluorescence. Besides, the complexes can be separated from cells by attaching biotin to them so that their enzymatic roles are identified. Details will be described in the presentation.

Poster Presentation : **LIFE.P-185**
Life Chemistry
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Structural Basis for the Psychrophilic Adaptation of Cold Shock Protein from *Colwellia psychrerythraea*: Tyr51 in the Hydrophobic Core

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Cold shock proteins (Csps) play key roles in the cold adaptation of bacteria. They function as RNA chaperones that destabilize structured regions in mRNAs, which are formed at low temperatures and induce fatal terminations of transcription. Here, we investigated the structure and dynamics of the psychrophilic Csp from *Colwellia psychrerythraea* 34H (*Cp*-Csp) for the first time. Despite of high sequence homology, its thermostability (37℃) was markedly lower than those of other Csps. NMR spectroscopic analysis revealed that *Cp*-Csp has a flexible structure with only one salt bridge and 10 hydrophobic core residues. Instead of the conserved Phe, *Cp*-Csp contains Tyr51 in its hydrophobic core. The Y51F mutation increased the stability of hydrophobic packing and may have allowed the formation of a K3–E21 salt bridge, increasing the thermostability to 43℃. *Cp*-Csp exhibited conformational exchanges in its ribonucleoprotein motifs 1 and 2, and these motions were decreased by the nucleic acid binding. Fewer salt bridges, longer flexible loops, and less compact hydrophobic cavity lead to the low thermostability of *Cp*-Csp. The conformational flexibility of *Cp*-Csp facilitates its accommodation of nucleic acids at extremely low temperatures in polar oceans and its function as an RNA chaperone for cold adaptation. (Lee, Yeongjoon, et al. (2018) *Biochemistry* 57(26), 3625-3640)

Poster Presentation : **LIFE.P-186**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Kinetic characterization of macrophage stimulating 1 receptor (MST1R) kinase inhibitors identified from kinase-focused library screening

Woosuk Choi, Jinho Lee*, Victor Sukbong Hong*

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Macrophage stimulating 1 receptor (MST1R), also called Recepteur d'Origine Nantais (RON), is a transmembrane tyrosine kinase present on the surface of various cells. MST1R plays an important role in regulating cell homeostasis such as cell proliferation, migration, survival and invasion. MST1R is highly expressed in various cancers such as prostate, breast, pancreatic, bladder, ovarian, lung and liver. Here we report on the identification and characterization of small-molecule inhibitors of MST1R kinase. Using the time-resolved fluorescence energy transfer (TR-FRET) assay technology, we performed screening of a kinase-focused library of 333 compounds at 10μM concentration and confirmed 27 compounds that effectively inhibited the activity MST1R. It was found that 3,5-disubstituted indolin-2-one structures were common cores in these hits. Kinetic analysis demonstrates that KMU010684, the most potent inhibitor from screening, was found to be competitive against ATP.

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Poster Presentation : **LIFE.P-187**
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The discovery of new MNK2 inhibitors using a homogenous time-resolved fluorescence resonance energy transfer (TR-FRET) assay

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The mitogen-activated protein kinase signal-interacting kinase MNK2 is a serine/threonine protein kinase that is a downstream target of the Erk and p38 mitogen-activated protein kinase (MAPK) pathways. MNK2 plays a critical role in its regulating eukaryotic initiation factor 4E (eIF4E) by phosphorylation and controlling mRNA translation. Many studies have identified that MNK2 is overexpressed in various cancer such as breast, prostate, head and neck, kidney and lung. Therefore, MNK2 is an important target for treating cancer. Using the time-resolved fluorescence resonance energy transfer (TR-FRET) assay, we screened human MNK2 with a kinase-focused library (333 compounds) and identified 20 hit compounds that effectively inhibited MNK2 activity. Of 20 hit compounds, the most potent compound KMU010903 (3,5-diamino-1,2,4-triazole) showed a competitive inhibition against ATP based on the mode of inhibition study.

Poster Presentation : **LIFE.P-188**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Amyloid fibril formation of α-synuclein by LOV2 protein in the presence of blue light

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The LOV(Light oxygen voltage)2 domain from Avena sative (AsLOV2) has an alpha helix (Jα) in the C-terminal which is bound to the central domain in the absence of light. Exposure LOV protein to blue light separates the Jα helix from the LOV core domain. We first carried out LOV2 subcloning to overexpress the LOV2 protein or LOV2-Syn fusion protein in E. coli. Upon induction by IPTG, LOV2 protein or LOV2-Syn fusion proteins were overexpressed and further purified. Their functions on modulation of amyloid fibril formation are discussed based on thioflavin T fluorescence assay.

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Poster Presentation : **LIFE.P-189**
Life Chemistry
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Molecular modeling of metal ion binding in zinc-ovalbumin nanocomposites as antimicrobial candidates

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We studied the binding of zinc ions to the protein ovalbumin (OVA). The synthesized Zn-OVA nanocomposites (NCs) have been comprehensively characterized in terms of their physicochemical properties and antibacterial activity. The antimicrobial assays showed that ZnO-OVA nanocomposites exhibit an inhibition effect against both bacteria (A. baumanii and K. pneumonia) and yeasts (C. albicans) strains. The final product and the binding process have been analyzed by spectroscopic and microscopic methods including X-ray diffraction (XRD), transmission electron microscopy (TEM), energy dispersive X-ray (EDX), and Fourier transform-infrared spectroscopy (FT-IR). Based on the kinetic studies, the Zn-OVA adsorption was described as a heterogeneous process consisting of three separate steps with the total efficiency of the process being ~65.12 ± 3.02%. The analysis of FT-IR changes before and after the Zn2+ binding to the OVA pointed out the crucial role of the deprotonated carboxyl and amid groups in the biosynthesis process of ZnO NCs. Additionally, both molecular dynamics (MD) simulations as well as quantum mechanics (QM) calculations were carried out in order to simulate and support the description of the protein-based ZnO nanocomposites formation mechanism. It was shown that the most prominent interacting amino acids with Zn2+ ions were aspartic and glutamic acid which was supported with DFT IR frequency calculations.

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Poster Presentation : **LIFE.P-190**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Simultaneous Detection of Multiple Pathogenic Targets with Novel Stem-tagged Primer Sets

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Simultaneous multiple gene detection is indispensable for the detection of various genes in a small sample obtained by an invasive method. A typical detection method is probe-based fluorescence melting curve analysis using real time PCR. It is very limited because a probe sequence must be designed with at least a different Tm for each target. To overcome this limitation, we developed a novel simultaneous multiple gene detection method based on a giant amplicon molecular beacon. PCR was performed by attaching stem sequences with different Tms to each primer set, and the melting Tm was measured by hybridizing the stem sequences at both ends of the amplified amplicon which generated well separated Tm signals. The important point here is that the stem sequence that produces the Tm signal is an arbitrary sequence that is not related to the target gene. Because it is an arbitrary sequence, the desired Tm can be freely adjusted. As a result, we succeeded in the simultaneous detection of four samples using only one fluorophore. Theoretically, a combination of five fluorophores could detect simultaneously more than 20 multiple genes.

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Poster Presentation : **LIFE.P-191**
Life Chemistry
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Phase diagram and motility of actins and microtubules on bulk; interaction and morphological aspects.

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The creation of cell-like structures, bottom-up biology, is an expanding research field that aims to understand the mechanisms of biological processes via assembly of their essential components in synthetic cells. The cytoskeleton in cell consists of three filamentous subsystems, microtubules, actin filaments and intermediate filaments. Microtubule and actin in cytoskeleton play an important role in cell migration, division and cell shape changes. Research on the interaction of microtubule and actin have been studied constantly and there are many opinions. Also, the research for imparting motility as living cells has been actively studied by using synthetic cytoskeleton. So, we tried to find clues for the interaction of actin and microtubule via the research for the phase diagram for actin polymerization, microtubule polymerization and actin-microtubule polymerization controlled with Mg2+ ion depending on Ca2+ concentration in a bulk. Also, to impart direction of polymerization for actin or microtubule fiber as control of cell motion controlled external chemical stimulation (Mg2+ ion), we fabricated patterned polymer including Mg2+ or Ca2+ ion, and then we could see the generation of actin or microtubule fiber on patterned polymer with Mg2+ or Ca2+ ion only. We will discuss the interaction and bundle mechanism of actin, microtubule, and actin-microtubule in a bulk. In addition, we will constantly study the imparting motility like live cell with polymerization of actin and microtubule controlled external chemical stimulation or with various scaffolds in artificial cell.

Poster Presentation : **LIFE.P-192**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Self-assembled DNA tetrahedron as a carrier for in vivo liver delivery of siRNA

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Self-assembled DNA nanostructures have been tested as carriers for delivery of many biologically functional molecules. In particular, self-assembled DNA nanostructures are ideal carriers for delivery of nucleic acid cargos because the cargo sequence can be incorporated into the DNA strands for self-assembly during the DNA synthesis, which abolishes the additional conjugation steps for cargo-loading. To develop DNA nanostructure capable of tissue-specific delivery of nucleic acids, we here attempted to use a DNA tetrahedron (Td) as a carrier for liver-specific delivery of siRNA in vivo. In this study, we showed that the siRNA delivered into liver by Td could down-regulate target mRNA sequence-specifically and lower the target protein level, suggesting that Td is a reliable carrier for in vivo liver delivery of siRNA.

Poster Presentation : **LIFE.P-193**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

SO82 serves as an inhibitor of protein-tyrosine phosphatase MEG2 relevant to insulin resistance

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Inhibition of PTP-MEG2 activity has been shown to be as a potential therapeutic strategy for the treatment of type 2 diabetes. Previously, we also have shown that PTP-MEG2 knockdown enhances AMP-activated protein kinase (AMPK) phosphorylation, suggesting that PTP-MEG2 can be a potential antidiabetic therapeutic target. In this study, SO82 inhibited the catalytic activity of PTP-MEG2 (IC50 = 32.47 μM) in vitro, indicating that it would be a potential antidiabetic candidate. Importantly, SO82 stimulated glucose uptake and led to enhanced phosphorylation of AMPK and Akt. Furthermore, SO82 did not accelerate adipocyte differentiation, suggesting that SO82 increased insulin sensitivity without significant lipid accumulation. Taken together, we demonstrated that SO82 as an inhibitor of PTP-MEG2 stimulated glucose uptake through activation of both AMPK and Akt signaling pathways. These results strongly suggest that SO82 could be used as a potential therapeutic candidate for the treatment of type 2 diabetes.

Poster Presentation : **LIFE.P-194**
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Structural and dynamic properties of type I human and type II bacterial acyl carrier proteins and their interactions with fatty acid synthesis proteins

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Department of Biotechnology, Konkuk University, Korea

Acyl carrier protein (ACP) is highly conserved small acidic protein and essential for the mammalian type I and bacterial type II fatty acid synthesis system by mediating acyl group delivery. To understand structural features of different types of ACP, we compared human ACP (hACP) and *Escherichia coli* (EcACP) by NMR spectroscopy. Analysis of chemical shift perturbations upon octanoyl group attachment showed that hACP does not sequester the acyl chain in the hydrophobic cavity, which is blocked by unique hydrophobic triad residues. Moreover, hACP showed more flexible backbone dynamics than EcACP, especially in the front of $\alpha_1\alpha_2$ loop. We further investigasted the interactions of hACP with *Streptomyces coelicolor* ACP synthase (ScAcpS), which is used to convert apo mammalian ACP to the holo form. Similar to protein-protein interface (PPI) found in hACP-hAcpS crystal structure, docking simulation and binding affinity measurements showed that the hydrophobic residues in universal recognition helix II of hACP contribute mainly to ScAcpS. In contrast, interaction found in EcACP-EcAcpS crystal structure is dominated by electrostatic interactions. These results suggest that ScAcpS has relatively relaxed substrate specificity and a similar charge distribution to hAcpS. These fundamental differences of the charge distribution in hAcpS, ScAcpS and EcAcpS largely affect the interaction with hACP. These findings can provide a useful resource for development of novel antibiotics inhibiting PPI in bacterial FAS proteins with specificity.

Poster Presentation : **LIFE.P-195**
Life Chemistry
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The Structure and Substrate Specificity of *Propionibacterium acnes* FAS proteins

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Acne vulgaris is characterized by inflammatory and non-inflammatory lesions, which are caused by the anaerobic gram-positive bacteria, *Propionibacterium acnes*. The fatty acid synthesis (FAS) is important for *P. acnes* and acyl carrier protein (*Pa*-ACP) and β-ketoacyl acyl carrier protein synthase III (*Pa*-KAS III) are an essential part of its FAS. In this study, we determined the structures and investigated the substrate specificities of *Pa*-ACP and *Pa*-KAS III. Solution structure of *Pa*-ACP revealed to have four α-helices (helix I, I7-T19; helix II, S40-F54; helix III, D60-N65; helix IV, V69-H79) connected by three loop regions. *Pa*-KASIII has wide pockets so it appears to be able to accommodate branched chain acyl-CoA. Conformation-sensitive urea polyacrylamide gel electrophoresis and tryptophan fluorescence quenching experiments confirmed that *Pa*-KAS III prefers isobutyryl-CoA as the acetyl-CoA. The ^{1}H-^{15}N HSQC spectra of holo and isobutyryl *Pa*-ACP also showed that it accommodate the branched-chain to its hydrophobic pocket. Biochemical characterization confirms *Pa*-ACP and *Pa*-KAS III comply with incorporation of branched-short chain CoAs. Based on these data, we will design inhibitors of *P. acnes* FAS protein as a novel antibiotic against *P. acnes* infection.

Poster Presentation : **LIFE.P-196**
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Sequestering ATP inside Mitochondria by Nucleopeptide inducing Cancer Cell death

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Adenosine triphosphate (ATP) has important roles in cellular processes such as energy production, cellular respiration, cell signaling and metabolism. Most of cancer cells have three times higher concentration of ATP compared to normal cells. By removing ATP inside cancer cells, it can result in severe effect such as apoptosis. Herein, we developed selective cancer treatment by sequestration and self-assemblies of ATP with nucleopeptide (NP). NP has nucleobase (thymine, thy) which interacts with adenine and alternative positively charged amino acids and hydrophobic amino acids which are mitochondria targeting sequence and it can self-assemble in water. NP exhibits higher binding affinity with ATP by electrostatic interaction and hydrogen bond resulting in large complex and assemblies with ATP compared to ADP. To enhance selectivity towards cancer cells, NP-ADP having nanometer-sized micelles accumulates inside cancer cells and form large assembly with ATP which has higher binding affinity by reversible interaction. Thus, sequestration of ATP and large assemblies of NP-ATP inside mitochondria cause severe effects such as the metabolic process of ATP and stress by structures towards cancer cells.

Poster Presentation : **LIFE.P-197**
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Purification and Biochemical Characterization of homoserine dehydrogenase from Peudomonas aeruginosa and Bacillus subtilis

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Homoserine dehydrogenase(HSD) catalyzes reduction of L-aspatate-4-semaldehyde to homoserine or oxidation reversely, which belongs to branch of aspartic pathway that making amino acid such as threonine, isoleucine, methionine. HSD has inteterst in industrial application since its important role at production of L-lysine. And it has been target of pesticides and antibiotics against pathogens. In this study, HDH from Pseudomonas aeruginosa (PaHSD) and Bacillus subtilis (BsHSD) were overexpressed in E. coil cell and purified to homogeneity for biochemical and biophysical characterization. Reverse direction was studied in kinetic assay. The enzymatic activity of both are maximal at pH 9.0. PaHSD exhibits preference both NAD+ and NADP+ ,while BsHSD shows its activity with NADP+ exclusively. And both are solved in highly concentrated NaCl solution. Enzymes exist in 4-meric state. In the CD study, it has similar curve with curve of another species and moderate thermostability resulting 50.82℃ of Tm. Attempt of crystallizing both enzymes is encluded in this study, while it is not published yet. The biochemical and biophysical characteristics of enzymes revealed in this study provide the basis for studies on the relationship between its structure and function.

Poster Presentation : **LIFE.P-198**

Life Chemistry

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Anticancer effects of a small organic compound with inhibition of Importinβ1 binding with transcriptional factor NF-κB.

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Nuclear Factor κB (NF-κB) is a protein complex comprised by various subunits and most common form is the p50 and p65(Rel A). NF-κB works as a transcriptional factor and occurs a cancer initiation in human. The subunit p65 of NF-κB is known that transferred by karyopherin beta 1 (KPNB1) one of transport protein from cytoplasm to nucleus. So, we conformed that NF-κB stronger bind to KPNB1 than karyopherin alpha (KPNA) another transport protein and showed binding affinity of KPNB1 with NF-κB to obtain kinetic values and inhibition effect by a small organic compound (compound 1) has an anticancer effect. Also, we analysis the NF-κB(p65) expression level using western blot analysis in H1299 and HeLa cancer cells with compound 1 to compare importin β1-specific inhibitor importazole (IPZ).

Poster Presentation : **LIFE.P-199**

Life Chemistry

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Synthesis of 2-aminothiazole derivatives with EGC as a anticancer compound

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(−)-Epigallocatechin (EGC) is one of the major flavonoid of green tea and has been studied anti-infective, anti-inflammatory, anti-cancer, and neuroprotection. Also, EGC strongly inhibits the growth of breast cancer cells (MCF-7 and MDA-MB-231), but the growth of normal breast epithelial cells does not. in addition, as shown that previous study 2-Aminothiazole derivatives have been shown to inhibit the actions of KPNB1. As a result, the cargo proteins that bind to the same sites of 2-Aminothiazole derivatives among the various cargo proteins carried by KPNB1 to the nucleus could not be transported, resulting in anticancer effects. Therefore, we would like to determine how the compounds of EGC and 2-aminothiazole derivatives affect KPNB1 in breast cancer cells.

Poster Presentation : **LIFE.P-200**
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Phloretin is a natural TLR2/1 inhibitor suppressed TLR2-mediated pathway

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Phloretin is a naturally occurring dietary flavonoid that is abundant in fruit. Here, we investigated whether the anti-inflammatory activity of phloretin is mediated through TLR2 pathways, and whether phloretin acts as an inhibitor of TLR2/1 heterodimerization. We tested the effects of phloretin on TNF-α production induced by various TLR-specific agonists. Phloretin significantly inhibited Pam3CSK4-induced signaling in Raw264.7 cells compared to TLR signaling induced by the other agonists tested. We further tested the effects of phloretin in HEK293-hTLR2 cells induced by Pam3CSK4, and confirmed that phloretin has comparable inhibition of TLR2/1 heterodimerization. Moreover, phloretin reduced the secretion of the inflammatory cytokines TNF-α and IL-8, whereas it did not significantly reduce these cytokines in cells. Western blot results showed that phloretin significantly suppressed Pam3CSK4-induced and NF-κB p65 expression. The molecular interactions between phloretin and TLR2 were investigated using bio-layer interferometry and in silico docking. Phloretin bound with micromolar binding affinity, and we proposed a binding model of phloretin at the TLR2–TLR1 interface. Overall, we confirmed that phloretin inhibits the heterodimerization of TLR2/1, highlighting TLR2 signaling as a therapeutic target for treating TLR2-mediated inflammatory immune diseases.

Poster Presentation : **LIFE.P-201**
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Design of 12-meric antimicrobial peptide analogs derived from Papiliocin for Gram-negative sepsis

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papiliocin, isolated from the swallowtail buterfly Papilio Xuthus, shows low toxicity and high bacterial cell selectivity particularly Gram negative bacteria. Papiliocin have Trp2 and Phe5 aromatic residues in N-terminal. Tertiary structures have revealed that these residues are generally composed of an N-terminal amphipathic α-helix and a hydrophobic C-terminal α-helix linked by a hinge in our previous studies. We determined the essential length of the N-terminal fragment of papiliocin necessary to retain its biological activity. The minimum inhibitory concentration values and cytotoxicity measurement revealed that a PapN-12mer containing a three-turn, amphipathic helix was the shortest peptide exhibiting antibacterial activity without cytotoxicity. Based on these results, we designed 12mer peptides derived from original sequence, to obtain more potent activity against multidrug resistant Gram-negative bacteria and to improve cell selectivity and anti-inflammatory properties. Especially, p12-6 peptides showed significant antibacterial activity as well as anti-inflammatory activities in vitro and in vivo, implying the potency to further develop as an anti-sepsis drug candidate.

Poster Presentation : **LIFE.P-202**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Transcriptome-wide identification of L1TD1-target RNA interactions in human embryonic stem cells

Young-Soo Kwon

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LINE-1 type transposase domain containing 1 (L1TD1) is one of the top genes specifically expressed in human embryonic stem (hES) cells. The RNA-binding protein L1TD1 is rapidly downregulated in response to differentiation. L1TD1 is required for self-renewal of undifferentiated hES cells and cancer cell proliferation. Therefore, L1TD1 is a potential target of anticancer drug discovery. Although the transcriptional regulators of pluripotency are extensively studied, the role of post-transcriptional regulators is still poorly characterized. To better understand functions of L1TD1, we have determined direct interactions between L1TD1 and RNAs in hES cells by using crosslinking immunoprecipitataion (CLIP) coupled with next generation sequencing. RNAs enriched by CLIP for L1TD1 map not only in genic regions but also in intergenic regions. The interacting RNAs mapping in annotated genic regions are located in introns and exons. L1TD1 binds RNAs transcribed from human-specific L1 long interspersed nuclear elements. KEGG pathway enrichment analysis reveals that L1TD1 binds mRNAs encoding proteins involved in Herpes simplex virus 1 infection, the majority of which are KRAB-zinc finger proteins. KRAB-zinc finger proteins are considered to be the cellular components of an arms race against transposable elements. Our results suggest that L1TD1 is implicated in regulation of transposition through direct binding to RNAs from transposable elements and binding mRNAs encoding zinc finger proteins that block transcription from transposable elements and resistance to viral infection.

Poster Presentation : **LIFE.P-203**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Global analysis of RBM39 protein-RNA interactions in human embryonic stem cells by CLIP-seq

Young-Soo Kwon

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RNA splicing is a fundamental process of eukaryotic gene expression and interactions between RNA molecules and RNA-binding proteins (RBPs) play essential roles in gene expression regulation by RNA splicing. Alterations of these proteins are also implicated in several human genetic diseases, including multiple cancers. RBM39 is a U2AF65-related splicing factor that was recently identified as the specific target of anticancer sulfonamides. However, RNA targets and functions of RBM39 are largely unknown. Systematic investigation of the RNA interaction maps of U2AF65 and RBM39 and their potential overlapping and distinct functions in splicing are an important question. Here, we present an interaction map between RBM39 and RNAs in human embryonic stem cells by using crosslinking immunoprecipitataion (CLIP) coupled with next generation sequencing. The majority of binding sites are located in splicing accepters that overlap binding sites of U2AF65. However, binding sites of RBM38 are limited to a small subset of splicing acceptors. KEGG pathway enrichment analysis reveals that RBM39 binds mRNAs encoding proteins involved in splicing regulation. Limited target sites may explain why RBM39 depletion by anticancer sulfonamide treatment specifically kills cancer cells that require high expression levels of splicing factors.

Poster Presentation : **LIFE.P-204**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

CRISPR-Cas9 system modifies the gene sequence of MITF transcription factor modulating melanin synthesis

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Melanin production was stimulated by several factors such as nitro oxide, α-MSH (α-melanocyte stimulated hormone), stem cell receptor in human melanocyte. The cause of hair graying has not been clearly elucidated, but the accumulation of hydrogen peroxide in the hair follicles and the decrease in the number of melanocytes have known to be involved in the reduction of melanin production. Microphthalmia-associated transcription factor (MITF) is considered a 'master regulator' of melanocyte development, differentiation and melanin synthesis. MITF also acts as a transcription factor for melanogenesis by promoting the protein expressions of tyrosinase, TRP-1, and TRP-2 which are important enzymes for melanin synthesis. Therefore, MITF gene knockout melanocytes were generated using the CRISPR-Cas9 gene editing system. The base substitution and deletion in the MITF gene sequence were confirmed by T7 endonuclease 1 assay and DNA sequencing analysis. It was also found that there was the difference between MITF gene mutated by CRISPR-Cas9 system melanocytes and normal melanocytes in the gene expression related to melanin synthesis modulated by MITF transcription factor in RT-PCR assay. Moreover, the protein expression in MITF gene mutated by CRISPR-Cas9 system melanocytes involved in melanin production was regulated by MITF transcription factor in western blot analysis and immunofluorescence staining. These results suggest that the CRISPR-Cas9 system could contribute to the elucidate identification of melanogenesis mechanism modulated by MITF transcription factor.

Poster Presentation : **LIFE.P-205**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Antidiabetic effect of DH047 and DH049 dual-targeting of protein tyrosine phosphatases

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Type 2 diabetes mellitus (T2DM) is a disease characterized by insulin resistance. Insulin resistance has a feature of defects in insulin signaling and several protein tyrosine phosphatases (PTPs) involved in this signaling pathway can be potential antidiabetic targets. We have screened natural compound isolated from a certain plant to identify potent inhibitors of PTPs involved in insulin resistance. Among them, DH047 and DH049 was selected as a dual-targeting inhibitor of PTP1B and SHP2. Then, we examined its IC_{50} and cooperative binding through evaluating hill coefficient in vitro. In 3T3L1 adipocytes, DH047 and DH049 increased GLUT4 translocation to the plasma membrane protein and stimulates glucose uptake in a concentration-dependent manner. In addition, DH047 and DH049 didn't increase the lipid components and adipogenesis in 3T3-L1 cells. Thus, these results suggest DH047 and DH049 is a potential therapeutic candidate for T2DM.

Poster Presentation : **LIFE.P-206**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

MITF and IGF-1 signaling pathways are involved in the aging of human melanocytes

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[1]*Department of Applied Chemistry, Dong-Eui University, Korea*

The aging of melanocytes has been known to be caused by the accumulation of H2O2. Previous study reported that hair graying is caused by H2O2, one of the reactive oxygen species. Therefore, the aim of this study is to investigate the effect of H2O2 on human melanocytes. The scavenging activity of intracellular H2O2 in both senescent and aged cells induced by H2O2 was reduced compared with young cells in DCFH-DA fluorescence assay. In addition, melanin synthesis was reduced in cells treated with H2O2 at 125 μM or more. Both the senescent cells with 40 of population doublings and aged cells induced by H2O2 showed higher expression levels of MSRA, MSRB, glutathione reductase, SOD-1 and catalase than young cells with 5 of population doublings in western blot. Furthermore, the expression levels of TRP-1, TRP-2 and p300 were reduced in both senescent cells and aged cells induced by H2O2 compared with young cells. However, the expression level of SIRT-1 was increased in both senescent and aged cells induced by H2O2 compared with young cells. The expression levels of (phosphoinositide 3-kinases) PI3K, v-akt murine thymoma viral oncogene homolog 1 (AKT1), mammalian target of rapamycin, β-catenin (CTNNB1), acetylated p53 (ac-p53), p53 and p-p21 proteins, related to IGF-1 and p53 signaling pathways, were higher in senescent and H2O2-treated cells than those of young cells. Furthermore, AKT reduced melanogenesis through microphthalmia-associated transcription factor (MITF) inactivation by the inhibition of CTNNB1. Above findings suggest that H2O2 is involved in the aging process of melanogenesis by the inhibition of melanin synthesis, and p53 protein plays a key role in the aging of melanocytes via IGF-1 signaling pathways.

Poster Presentation : **LIFE.P-207**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Identification of KDH02 and Baicalin synergy effect for obesity treatment

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Obesity has been cited as a contributing factor to approximately 100,000–400,000 deaths in the United States per year and has increased health care use and expenditures. It is a serious health issue that can cause numerous diseases such as metabolic syndrome including heart disease and high blood pressure, atherosclerosis, type 2 diabetes, high blood cholesterol, cancers and sleep disorders. The cause of obesity is the increasing number and size of fat cells in the body. Treatments include lifestyle changes, such as heart-healthy eating and increased physical activity, and Food and Drug Administration (FDA)-approved weight-loss medicines. Baicalin, isolated from the genus Scutellaria, reported several times with a bioactive agent of biological activities including anti-adipogenesis. The multi-treat of KDH02 and Baicalin may have a synergy therapeutic effect against obesity. To identify the effect of KDH02 and Baicalin in the treatment of obesity, we evaluated its biological activities in 3T3-L1 adipocytes to demonstrate its possibility for anti-obesity drug. These results identify potential new therapeutic strategies for obesity treatment.

Poster Presentation : **LIFE.P-208**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Cell-Free Expression in Giant Unilamellar Vesicle with Phase Separation by Emulsion Transfer Method

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

Giant Unilamellar Vesicle (GUV) is a promising model to study cell and its internal or extracellular systems. To mimic the real cell, it contains an aqueous environment surrounded by a versatile and asymmetric boundary mainly made of phospholipids and membrane proteins. Ideally, the aqueous environment should provide a confined space with sufficient components for various enzymatic reactions inside the vesicle. However, it is notoriously challenging to reach that minimal but optimal status in artificial cell construction. Here we aim to create GUVs with Lo/Ld (Liquid Ordered/ Liquid Disordered) phase separation (LPS) and apply this model to examine cell-free expression inside GUVs. Instead of using the popular electroformation method, we employ Emulsion Transfer Method (ETM) by using Water-in-Oil emulsion and expect to observe the difference in protein expression which can lead to change in morphology of our LPS-GUVs, compared to vesicles without LPS.

Poster Presentation : **LIFE.P-209**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

NMR Dynamics Study of DNA Binding Domain of Transcription Factor MEIS1

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Transcription factors are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. Homeobox genes, of which the most well-characterized category is represented by the HOX genes, play a crucial role in normal development. MEIS1 (myeloid ecotropic viral insertion site 1) is a viral integration site in murine myeloid leukemia cells. This gene encodes a homeobox protein belonging to the TALE ('three amino acid loop extension') family of homeodomain-containing proteins. TALE proteins are distinguished by the presence of three extra amino acids in the loop binding the first to the second alpha helix of the homeodomain. he highly conserved DNA-binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif, [5'- TGACA- 3']. Further DNA-binding specificity within TALE family members is determined by adjacent DNA sequences and through the binding of additional transcriptional partners. We performed $^{1}H/^{15}N$ HSQC experiment and imino proton NMR experiments between MEIS1 and consensus MEIS1 target DNA (msDNA). The exchange rate constants of the imino protons for the wild type and mutant were measured by using water magnetization experiment. We compared to the binding affinity of MEIS1 for both wild type and mutant and characterized its target DNA recognition.

Poster Presentation : **LIFE.P-210**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Optimization of loading hydrophobic fluorescent probes within F127 sIPN

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Department of Chemistry, Pukyong National University, Korea

We present a method to efficiently stabilize micelles of F127 by semi-interpenetrating network (sIPN) formation. First, pentaerythritol tetraacarylate (PETA) loaded in the core was crosslinked to form sIPN resulting in stabilized particles against temperature and concentration changes. We characterized size and stability of the particles by fluorescence, UV-Vis spectroscopies, and dynamic light scattering. In addition, rheological behavior of the particles was investigated by large amplitude oscillatory shear. The resulting nanoparticles were able to incorporate both organic and inorganic hydrophobic fluorescent probes. Furthermore, a number of chemical compositions and experimental conditions were tested to optimize sIPN formation of the polymer.

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Poster Presentation : **LIFE.P-211**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Administration of functional DNA nanoparticle for cancer immunotherapy

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[1]*Shanghai Public Health Clinical Center, Fudan University, Korea*

Nucleic acids are one of basic components for living organisms. At the same time, DNAs and RNAs can be used as building blocks to build nanostructures using the sequence specific selfrecognition. The incorporation of lipid-modified nucleotides into DNA strands enables the formation of nano-size micelles. In a single self-assembly step, the micelles can be equipped with an immune adjuvant (CpG motifs) and an antigen peptide (OVA epitope) bearing peptide nucleic acid (PNA). In past research, we observed dose-dependent (CpG) activation of TLR-9 resulting in DC maturation in vivo. Here, we report the effect of the immunotherapeutic nucleic acid (INA) including immune-adjuvant and antigen peptide on the surface of lipid-modified DNA micelles in inhibition of melanoma tumor growth and its metastasis in the mouse model.

Poster Presentation : **LIFE.P-212**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of O-Acylated Shikonin derivativesto discover adipogenic inhibitors

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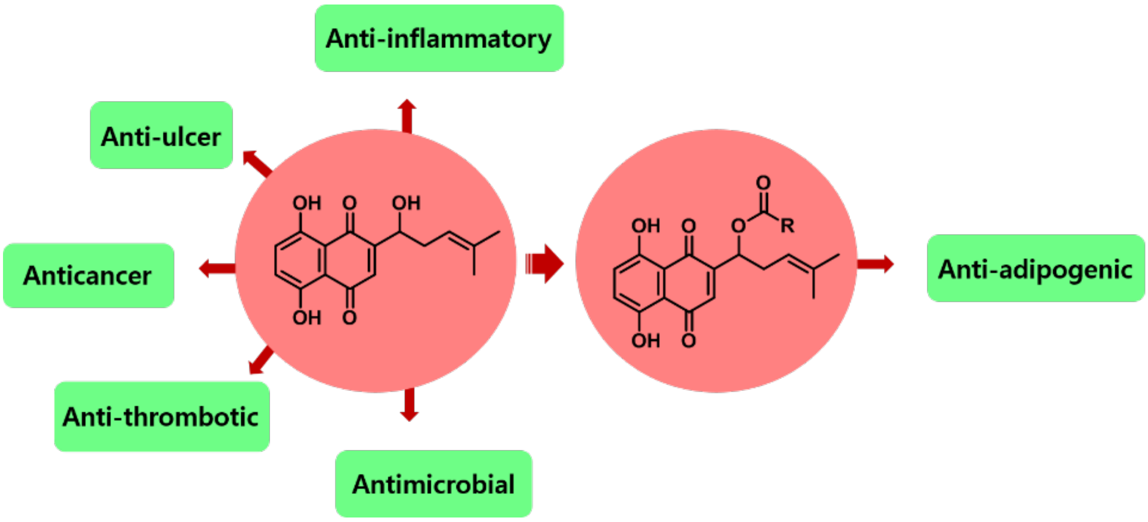
[2]*School of Pharmacy, SungKyunKwan University, Korea*

Shikonin is a natural dye which has been used for food coloring and in cosmetics because of the strong red color. Shikonin is extracted from the root of Lithospermum erythrorhizon, commonly called red gromwell, and is widely used in Asian cultures as an herbal medicine. Various biological activities of Shikonin are known, including anti-ulcer, anti-thrombotic, antimicrobial, anti-inflammatory, and anticancer activities. Furthermore, it also displays anti-adipogenic effects1. Previous study showed that shikonin inhibits adipogenic differentiation by blocking the ERK signaling pathway during the early stages of adipogenesis thereby preventing high fat diet induced obesity in mice2. Interestingly, acylation of the secondary alcohol of shikonin leads to a significant increase in its diverse activities. Here, we present the synthesis of several acylated shikonin derivatives in an attempt to discover a shikonin derivative with improved anti-adipogenic effect.


Anti-inflammatory
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Poster Presentation : **LIFE.P-213**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and application of peptide libraries using unnatural amino acids

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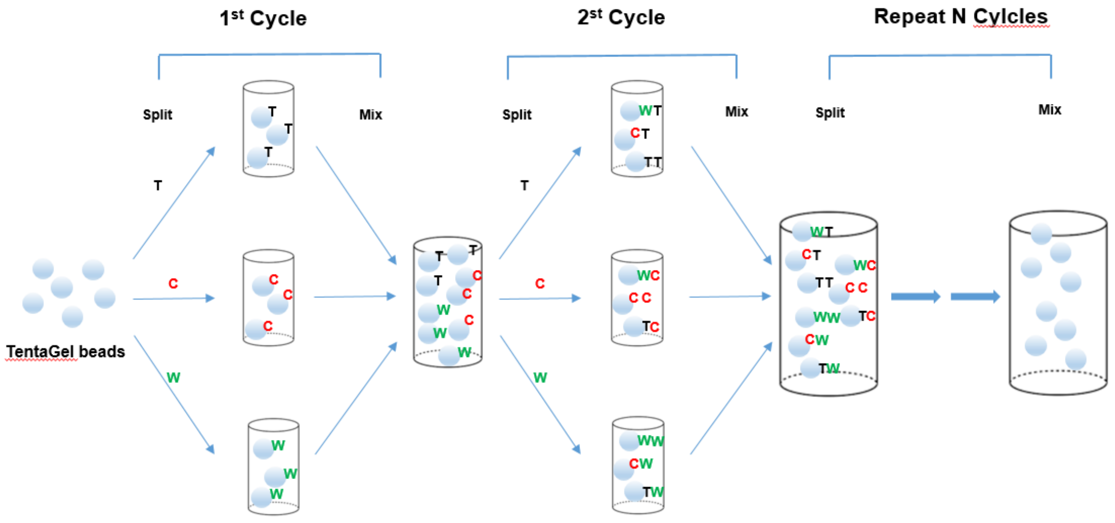
The design and synthesis of unnatural amino acids is growing rapidly as the demand for potential therapeutics and other diversified novel functional applications increases. To this end, we synthesized unnatural amino acids with diverse moieties that can selectively bind to a specific protein, and applied them in the preparation of peptide libraries.To construct the peptide libraries, we used a one-bead one-compound (OBOC) combinatorial library approach. Screening of OBOC libraries is widely used to identify ligands with desired pharmacological properties, for analytical applications, and to purify or detect proteins in complex mixtures.The aim of our study is to obtain peptide libraries containing unnatural amino acids and to discover novel peptide sequences that can bind to specific target protein.



Poster Presentation : **LIFE.P-214**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Photostable polymeric nanoparticle containing hydrophobic Lumogen® dye as cellular biomarkers

Mingyeong Kang, **Minseok Kwak***

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Lumogen fluorescent dyes have great light stability as well as high fluorescence quantum yields. Despite the excellent photophysical properties of dyes, the highly hydrophobic structure in common makes the compounds difficult to function as biological fluorescence probes. To generally utilize a family of organic fluorescent dyes such as Lumogen Red, Orange, Yellow, and Violet, as a biomarker for cellular imaging in flow cytometry and fluorescence microscopy, we used an encapsulation method using amphiphilic block copolymer namely Pluronic F127. The photostability of Lumogen nanoparticles were compared with commercial dye, Alexa488 and DAPI, used primarily bioimaging. Cell uptake of the probe nanoparticles by HeLa cells was analyzed by flow cytometry and confocal laser scanning microscopy. Also, we observed to confirm the position of the Lumogen nanoparticles in the HeLa cells using a high voltage electron microscope.

Poster Presentation : **LIFE.P-215**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A bioorthogonal turn-on fluorescent strategy for post-synthetic modification of DNA

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Fluorescent labelling by bioorthogonal chemistry is an attractive tool for imaging of nucleic acids. Most post-labeling methods using commercial fluorescent materials are signal-to-noise ratio limited due to remaining unreacted labeled fluorophores. Here, we report a primary amino-selective fluorescence turn-on method for post-labelling DNA using non-fluorescent ylidenmalononitrile enamines. Oligonucleotide containing primary amine functional unit was synthesized through solid-phase synthesizer with 5´-protected propargylamino-deoxyuridine phosphoramidite. Fluorescence spectra, MALDI-TOF mass spectrometry, and autoradiograms were recorded to confirm the primary amino-selective fluorescence turn-on in the oligonucleotides when using the three different ylidenmalononitrile enamines (P1, P2, P3). Among these compounds, P3 exhibited the strongest fluorescence signal when reacting with amino-oligonucleotide. Interestingly, P3-labelled oligonucleotide shows dramatic changing of fluorescence property depending on pH. It also provided a dramatic time-dependent fluorescence turn-on signal without any washing steps. Moreover, we demonstrated post-labeling reaction in cellular environment with the excellent signal-to-noise ratio. With dual emission fluorescent property, P3 is a promising candidate for high-resolution molecular imaging. Live-cell imaging experiments demonstrate the application potential of this new turn-on fluorescent bioorthogonal reaction.

Poster Presentation : **LIFE.P-216**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

N-Arylation of Adenosine: A Divergent Approach from Nucleoside to DNA

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Here in we report an efficient metal free N- arylation of adenosine with ortho/para electron-withdrawing group containing fluoroaryls using K3PO4 as base under mild reaction conditions. The obtained 6N-arylated nucleoside derivatives display bluish-green turn-on fluorescence, as a resultant by the effective adenosine push - pull system. Amongst, the adenosine - p-benzonitrile, appears to be highly fluorescent with QY- 0.102. We further demonstrated this methodology on various AT-rich oligonucleotides (DNA) containing one, two and three adenosine moieties. To the best of our knowledge, we have developed a first direct transition metal free N-arylation of nucleosides and oligonucleotides under mild condition at biologically ambient temperatures. This method features a new direct inexpensive route for fluorescence labeling of commercial oligonucleotides under ambient conditions.

Poster Presentation : **LIFE.P-217**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

EXTRACELLULAR MATRIX PROTEIN DELIVERY SYSTEM FOR TISSUE REGENERATION

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

Wound healing is an essential physiological process in which tissue repair and regeneration occur after injury1. The lack of several factors for wound healing such as growth factors and extra-cellular matrix (ECM) has been observed in hard-to-heal wounds2. Drugs developed from growth factors failed to provide expected outcome; therefore, ECM proteins approach is emerging as a promising alteration3. Human neonatal dermal fibroblasts HNDF was used for in vitro experiments. Either pure liposomes, fibronectin or fibronectin coated on liposomes were delivered to the cells. WST-1 cell proliferation assay and fluorescence live-cell imaging were performed to evaluate cell growth and migration in each group. Mouse model of ulcerative colitis induced by acetic acid was used for in vivo experiments. HE staining of the colon tissues and measurement of inflammatory cytokines level were performed in our study. We found a significantly faster growth in the cells after three day treated with liposomes coated by fibronectin (FN) compared to FN merely dissolved in media. Moreover, in in-vitro scratch assay, this group has remarkably shorter recovery time the control group. In vivo data confirmed that the mice with intestinal ulcers were observed with less tissue damage when treated with treated with FN-coated liposomes than other groups after 10 days. Our results revealed that fibronectin, when coated to liposomes prior to delivery to cells, can change FN structure and therefore have significantly higher effect in wound healing than when delivered with no carrier. This is promising to develop a wound healing material using our SUV-based ECM delivery system.REFERENCES: 1Takeo, M.; Lee, W.; Ito, M., Wound healing and skin regeneration. Cold Spring Harb Perspect Med 2015, 5 (1), a023267. 2Sawicka, K. M.; Seeliger, M.; Musaev, T.; Macri, L. K.; Clark, R. A., Fibronectin Interaction and Enhancement of Growth Factors: Importance for Wound Healing. Adv Wound Care (New Rochelle) 2015, 4 (8), 469-478. 3Dinh, T.; Braunagel, S.; Rosenblum, B. I., Growth factors in wound healing: the present and the future? Clin Podiatr Med Surg 2015, 32 (1), 109-19.

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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **LIFE.P-218**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Application of bacterial expression system and an amphipathic polymer to characterize mechanosensitive channel, tentonin-3

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[1]*Department of Bionano Chemistry, Kookmin University, Korea*

Tentonin-3 is known for a mechanosensitive channel protein which responds to membrane tension by mechanical stimuli. To establish efficient purification condition of tentonin-3 in E. coli, recombinant tentonin-3 was designed by using P9 sequence. An envelope protein of phi6 phage, P9, was fused to the N terminus of tentonin-3 and followed by His6 to the C terminus. The recombinant tentonin-3 was expressed in the membrane fraction of BL21star(DE3)-pRARE. Using Ni-NTA affinity chromatography and size-exclusion chromatography, we purified P9-tentonin-3 in homogeneity. The purified P9-tentonin-3 was stabilized by amphipathic polymer, APG, and reconstituted into LUVs. Reconstitution of the Tentonin-3 into liposome by APG showed higher efficiency than detergent mediated reconstitution method. In this condition, channel opening mechanism of tentonin-3 has been investigated by using various method of mechanical stimuli.

Poster Presentation : **LIFE.P-219**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Functional expression of human prostaglandin e2 receptor 4 (EP4) in E. coli and characterization of the binding property of EP4 with G alpha proteins

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[1]*Kookmin University, Korea*

EP4 is a receptor of prostaglandin E2 (PGE2) and belongs to rhodopsin-type GPCR family. The EP4 receptor is expressed in various tissues cells, including the immune, cardiovascular, gastrointestinal and respiratory systems and various cancer cells. EP4 mainly coupled with stimulatory G protein, and activate PKA resulting the increase of intracellular cAMP level. In this study, a recombinant protein consisting human EP4 fused to the C-terminus of P9 protein, a major envelope protein of phi6 phage, was overexpressed in the membrane fraction of E. coli. The expressed protein, P9-EP4, was efficiently purified by Ni-NTA affinity chromatography and stabilized with amphiphilic polymers (APG) derived from poly-gamma-glutamate. The specific interaction between P9-EP4 and G protein alpha subunits was demonstrated. In addition, both the ligand (PGE2) and antagonist (ONO-AE3-208) of EP4 showed specific binding to P9-EP4. The functional EP4 prepared in this study could also facilitate the development of EP4-targeting drugs.

Poster Presentation : **LIFE.P-220**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Isolation of single-chain variable fragments about Lysophosphatidic acid receptor 2 (LPA2) using purified recombinant LPA2 as the target

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Kookmin University, Korea
[1]*Department of Bionano Chemistry, Kookmin University, Korea*

Lysophosphatidic acids (LPAs) are potent signaling molecules that influence diverse cellular responses such as cell proliferation, migration, cell survival, and pathological responses. LPA receptors belong to the G protein coupled receptor (GPCR) family, and seven subtypes of LPA receptors have been identified. Among them, LPA receptor 2 (LPA2) is involved in the proliferation and metastasis of ovarian and breast cancers. Hence, LPA2-specific antagonists or antibodies are considered as potential anticancer therapeutics. To develop antibodies against LPA2, the recombinant LPA2 was expressed in Escherichia coli and purified in homogeneous form. The purified LPA2 was stabilized with biotin conjugated amphiphilic polymers (biotin-APG). The stabilized LPA2 was immobilized on streptavidin magnetic beads or streptavidin coated immunoplates, and OPALS phage library displaying single-chain variable fragments (scFvs) was applied to select LPA2-specific scFv clones. After biopanning, a few scFv clones which showed specific binding to LPA2 were identified, and their binding properties to LPA2 had been characterized.

Poster Presentation : **LIFE.P-221**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Detection of Gram-negative bacterial outer membrane vesicles using DNA aptamers

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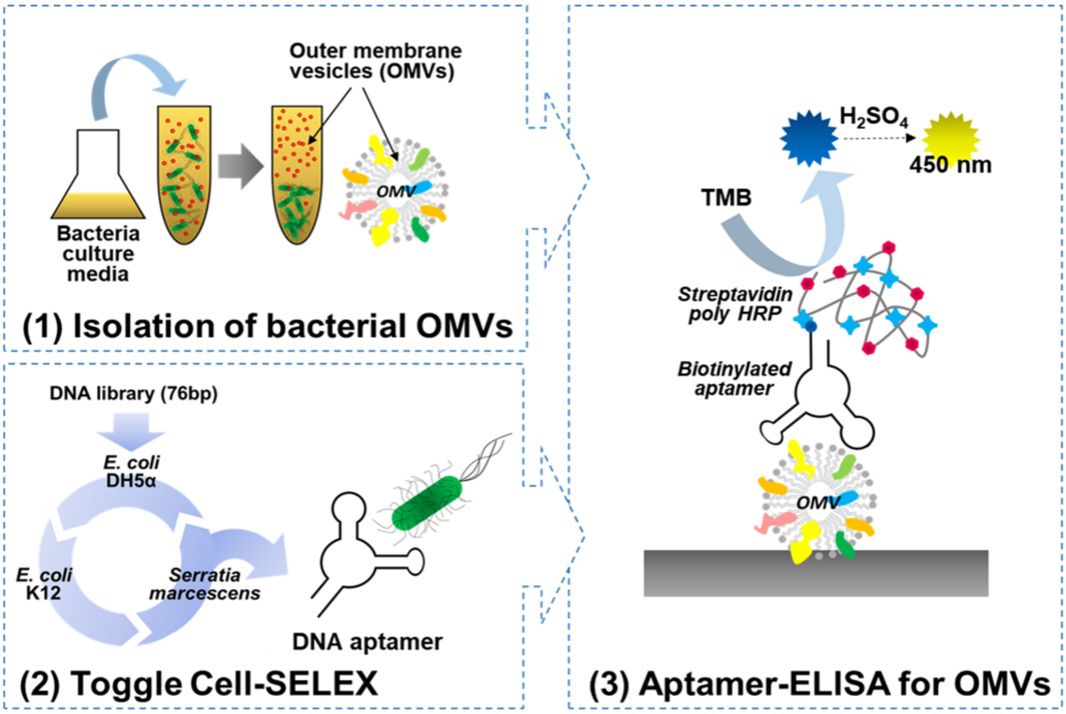
Infection of various pathogenic bacteria causes severe illness to human beings. Despite the research advances, current identification tools still exhibit limitations in detecting Gram-negative bacteria with high accuracy. In this study, we isolated single-stranded DNA aptamers against multiple Gram-negative bacterial species using Toggle-cell-SELEX (systemic evolution of ligands by exponential enrichment) and constructed an aptamer-based detection tool towards bacterial secretory cargo released from outer membranes of Gram-negative bacteria. Three Gram-negative bacteria, *Escherichia coli* DH5α, *E. coli* K12, and *Serratia marcescens*, were sequentially incubated with the pool of random DNA sequences at each SELEX loop. Two aptamers selected, GN6 and GN12, were 4.2-times and 3.6-times higher binding to 10^8 cells of Gram-negative bacteria than to Gram-positive bacteria tested, respectively. Using GN6 aptamer, we constructed an Enzyme-linked aptamer assay (ELAA) to detect bacterial outer membrane vesicles (OMVs) of Gram-negative bacteria, which contain several outer membrane proteins with potent immunostimulatory effects. The GN6-ELAA showed high sensitivity to detect as low as 25 ng/mL bacterial OMVs. Aptamers developed in this study show a great potential to facilitate medical diagnosis and early detection of bacterial terrorism, based on the ability to detect bacterial OMVs of multiple Gram-negative bacteria.


Outer membrane vesicles (OMVs)
Bacteria culture media
OMV
(1) Isolation of bacterial OMVs
DNA library (76bp)
E. coli DH5α
E. coli K12
Serratia marcescens
DNA aptamer
(2) Toggle Cell-SELEX
H_2SO_4
450 nm
TMB
Streptavidin poly HRP
Biotinylated aptamer
OMV
(3) Aptamer-ELISA for OMVs

Poster Presentation : **LIFE.P-222**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Quest for Eukaryotic Histone H4 Histidine Kinases

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

Protein histidine (His) phosphorylation and responsible His kinases (HKs) have been well characterized in bacteria (two-component systems; TCSs), while little is known about the HKs in eukaryotic cells. Although eukaryotic HK activities towards histone H4 has been reported over 40 years ago, with their potential involvement in cell proliferation, the identity of the kinase remains elusive. Here we report our progress towards the isolation and identification of HKs using chemical biology tools.References Besant, P.G & Attwood P.V., Biochimica et Biophysica Acta 2005, 1754(1-2), 281–290.

Poster Presentation : **LIFE.P-223**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Molecular dynamics simulations revealed a gating mechanism of nicotinic acetylcholine receptors

Myunggi Yi

Department of Biomedical Engineering, Pukyong National University, Korea

Nicotinic acetylcholine receptors (nAChR) are essential in neurotransmission. Although there are many research on the allosteric mechanism of ligand binding event triggering channel opening in transmembrane domain, the relationship between structure and function in atomic scale is still unclear. In this study, we focused on investigating the gating mechanism of nAChR through either apo form or ligand bound forms. We performed 4 molecular dynamics (MD) simulations of α4β2 nAChR: wild type of apo form (APO), acetylcholine bound wild type (ACH), wild type of BuIA toxin bound form (WT) and toxin bound mutant type (MT) α4β2 nAChR's whose 3 residues of α4 subunit (Tyr185, 187Asp and Agr188) replaced by 3 corresponding residues of α6 subunit. These three α6 residues are determinants of the toxin α-conotoxin BuIA selectivity of α6 subunit. The calculations of pore radii of the channels showed that the MT and APO forms had restriction radii of 1.9 and 2.3 Å (Glu261, Lys260 on beta subunit), while the same region was broadened in WT and in ACH (radii of 2.6 and 3.4 Å). The analysis of conformations showed that the asymmetric tilting motion of extra cellular domain (ECD) was observed in WT and ACH caused the asymmetric twist angle between ECD and TMD. This motion induced the asymmetrically arranged transmembrane domain (TMD) to become more symmetric. In contract, the opposite tendency was observed in MT and APO systems. In summary, we conclude that the inherent asymmetric arrangement of α4β2 nAChR can be broken by an unequally tilting motion of ECD and induce the symmetric arrangement in TMD, which makes the channel open.

Poster Presentation : **LIFE.P-224**

Life Chemistry

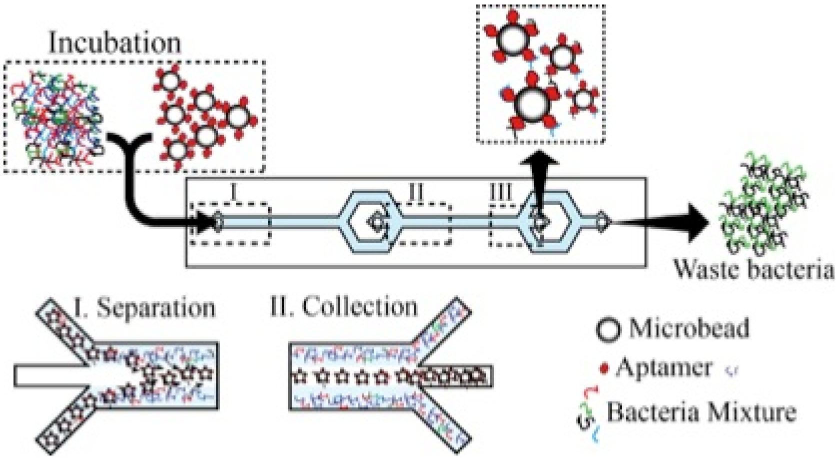
Exhibition Hall 1, FRI 11:00~12:30

Aptamer-bead mediated separation of gram-negative bacteria using microfluidic acoustophoresis

Byung Woo Kim, Dong-ki Lee[1,*]

Institute of Digital Anti-aging Healthcare, Inje University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Here, we demonstrated the development of microfluidic acoustophorsis device that enables the efficient and rapid separation of gram-negative bacteria from cultured media. Bacterial infections cause many detrimental risks due to their virulent factors. The gold standard for finding the causing pathogen in a blood sample is blood culture, which may take hours to days. Shortening the time to diagnosis would significantly reduce mortality. Our design enhances the separation efficiency by incorporating a lengthier, square shaped microchannel. Both inlets and outlets have a trifurcated junction, which makes simultaneous separation of the targets from a mixed sample possible by focusing the target particles at the center of the microchannel and the unwanted near the microchannel walls. From this architecture, the simultaneous excitation of two orthogonal resonances can generate 2-D acoustic standing wave by single piezoelectric actuation, focusing particles tightly on nodal points. Microbeads modified with a RNA aptamer,GN6, which has specificity to gram-negative bacteria were incubated with bacteria culture sample and then were injected into the acoustophoretic channel for simultaneous separation and washing. For the proof of principal, we tested separation performance of microfluidic acoustophoresis device using 10 different types of Gram-negative bacteria and 5 different types of Gram-positive bacteria. After separation of target bound bead using the device, we investigated and counted number of bacteria bound in each microbead in single bead observation manner. This protocol showed high specificity towards all Gram-negative bacterial as high sensitivity of as 103cells/ml of the bacterial and no (or limited) specificity of the Gram-positive bacteria.


Incubation
I
II
III
Waste bacteria
I. Separation
II. Collection
Microbead
Aptamer
Bacteria Mixture

Poster Presentation : **LIFE.P-225**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

NMR study of fusion protein Zα Domain of ADAR1 linked N-terminal domain of the vaccinia virus protein E3L

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Left-handed Z-DNA, which is a polymer of alternating d(CG)n sequence, is a higher energy conformation than B-DNA. Z-DNA is induced by high salt, negative supercoiling, and complex formation with Z-DNA binding proteins. Z-DNA binding domains are found in the RNA editing enzyme (ADAR1) and DNA-dependent activator of IFN-regulatory factor (DAI) in vertebrates, the E3L protein of poxviruses. Recent NMR studies of the complex formed between ZaADAR1 and a 6-base-paired (6-bp) DNA duplex referred to as d(CG)3, have suggested an active B–Z transition mechanism, in which the ZaADAR1 protein first binds to B-DNA and then converts it to left-handed Z-DNA, a conformation that is subsequently stabilized by the additional binding of a second ZaADAR1 molecule. All poxviruses have a gene called E3L that is essential for pathogenesis in the vaccinia virus. The E3L protein consists of two domains: an N-terminal Z-DNA binding domain and a C-terminal RNA binding domain. This N-terminal region shows sequence homology to the Za domains found in human ADAR1 (hZaADAR1). The Z-DNA binding affinity of the Za domain of E3L is required for viral pathogenicity. Here, to investigate the molecular mechanism of the B–Z transition of a DNA duplex induced by the fusion protein ZaADAR1+E3L(ZaA+E), we have conjoined a ZaADAR1 with ZaE3L and performed NMR hydrogen exchange experiments on the complexes formed by ZaA+E and d(CG)6 with a variety of protein-to-DNA (P/N) molar ratios. Comparison of these results with those from the analysis of hZaADAR1–d(CG)3 and ZaE3L-d(CG)3 in a previous study leads to valuable insights into the molecular mechanism of the B–Z transition of a DNA duplex induced by the fusion protein.

Poster Presentation : **LIFE.P-226**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Can the aqueous microdroplets work as reaction vessels for the building block of primitive lifeforms?

Hani Jeon, Sangmoon Lhee*

Center for Plant Aging Research, Institute for Basic Science, Korea

The micron-sized aqueous microdroplet provides peculiar physico-chemical environments enabling the accelerated reaction rates and modulating the thermodynamic values of reaction components. Although abiotic sugar phosphates and nucleosides synthesis are unfavorable in the bulk solution, such the reactions became favorable under the microdroplet environment, suggesting the microdroplet like cloud particles can work as synthesis reaction vessels for some biological materials. Here, we have tested the chain elongation of nucleotides and protein based on the microdroplet system.The elongation processes of DNA/RNA and protein chains are based on the condensation reactions of monomeric building blocks such as nucleotides and amino acids, which are exergonic (unfavorable) in aqueous solution. So, we observed the procedure of such the reactions in the form of the microdroplet. The elongation reactions of nucleotides and amino acids in the charged microdroplet is verified by high-resolution mass spectrometry. We expect that we can show a plausible physico-environment bearing the basic building blocks of primitive lifeforms through the microdroplet studies. Furthermore, these studies provide ultimate information about many biological reactions relating the aging processes of plants and animals, which happen inside the confined space like microdroplet. Keywords: Microdroplet, Electrospray ionization, Prebiotic chemistry

Poster Presentation : **LIFE.P-227**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A novel siRNA delivery complex using Cell-Penetrating Peptide (CPP)-Peptide Nucleic Acid (PNA) conjugates.

Prajwala Devarapalli, Yong Ho Kim[1,*]

Nanoscience and Technology, Sungkyunkwan University, Korea
[1]*Department of Chemistry, SKKU Advanced Institute o, Korea*

Effective and stable delivery of siRNA (small interfering RNA) into the cells require translocation of siRNA into the cytosol to treat multiple diseases. Several carriers have been employed to enhance the stability and efficiency of siRNA delivery. Considering their safety, efficiency, and targeting capabilities, cell-penetrating peptides can be the solution for overcoming the major obstacles in siRNA delivery. Another side, Peptide nucleic acid (PNAs) are DNA analogs, in comparison to nucleotides they have better chemical stability. In this study, we developed a novel delivery platform based on the CPP-PNA conjugates as a linker can be complexed with siRNA, where PNA called as a universal linker that is complementary to the part of siRNA but not sequence-specific. The complex formation was optimized by the stoichiometry of each component, confirmed by gel retardation assay. In vitro, the transduction efficiency of the complex was higher and cytotoxicity of the Peptide PNA conjugates did not show up to 20uM. The benefit of the system is not only cell penetration and allows better stability in serum environment to siRNA. Delivery efficiency and stability of the complex can expect high silencing activity. This new technology can greatly reduce difficulty and cost without a chemical modification and it can be an efficient approach for cell-specific delivery of siRNA.

Poster Presentation : **LIFE.P-228**

Life Chemistry

Exhibition Hall 1, FRI 11:00~12:30

NIR Emissive C2V Symmetric Pyridinium Salt: Selective Discrimination Capabilities G-Quadruplexes over Canonical/Non-Canonical Nucleic Acids and Their In-Cellulo Demonstrations

Anup Pandith

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G-quadruplexes (G4s) are non-canonical nucleic acids which can regulate various metabolic process in physiological systems. Due to its inevitable applications in genetics and therapeutics its recognitions in genome attracts great interest both chemical-biologists and genetic engineers. Considering the significance of G4s, current work we report small and highly efficient novel NIR emissive C2V symmetric pyridinium salt (1) was utilized to identify G4s in invitro as well as in in-cellulo. Rationally designed probe 1, showed selective switch-on response in NIR region (emission centred at 620 nm) without inducing any background signals from dsDNA, ssDNA, RNA and other non-canonical nucleic acids viz., triplex, three-way junction etc. Additionally, strategic design and sensing capabilities were supported through model compounds 2, 3 and 4 using UV-Vis, fluorescence, gel electrophoresis, and dynamic light scattering (DLS) studies.

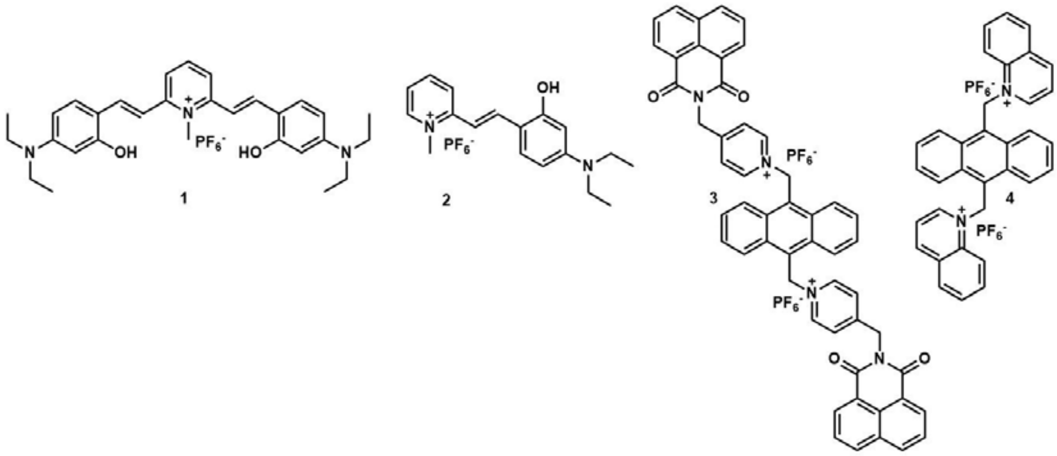

Fig. 1 Structure of fluorescent probes **1**, **2**, **3** and **4**.

Poster Presentation : **LIFE.P-229**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Proteogenomics Study for Identifying Cancer Biomarker Peptide Candidate with PTMs based on Novel Data Analysis Strategy utilizing Multi-Stage approach

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Center for Proteogenome Research (CPGR), Korea University, Korea
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Large-scale cancer genome sequencing studies have generated an extensive catalogue of mutations as disease biomarker and potential therapeutic targets. Difficulty in differentiating the driver and passenger mutations hurdles in the future development of drug targets hypothesis. Proteins are central to cellular functions, and mutated proteins can drive the initiation of tumor, progression and thereby act as targets to treatment. Proteomics enable an opportunity for functional interpretation of these mutations for better understanding of etiology of cancer development and thence target for therapeutic developments. Proteogenomics provide opportunities for protein level validation of genomic alterations guided by genomics data (RNA-Seq/Exome Seq). More than 300 different types of protein modifications have been described, many of which are known to have pivotal roles in cellular physiology. Protein and their PTM sites is key to dissection of PTM-mediated cellular processes and disease. Here we developed a sensitive method utilizing multi-stage database search for comprehensive proteomics data analysis to complement genomics sequencing data. We employed two complementary search engines, MS-GF+ and MODa/MODi here. The tandem MS data were first subjected to MS-GF+ database search (1st stage search) for mutation search using RNA-Seq guided sample specific mutated proteomics database (generated using CustomProDB) and the unidentified MS/MS data from the 1st stage search were analyzed with the combined use of MODa and MODi (2nd stage search), tools for blind and unrestrictive modification search using the same sample specific mutated proteomics database, respectively. When combined with mPE-MMR, a tool for accurate and extensive precursor masses assignments to co-fragmented MS/MS data, our method was shown to significantly increase the identification of peptides, post-translationally modified(PTMs) peptides, mutated peptides/genes. The developed method will be used for integrated cancer proteogenomic analyses. Keywords: mPE-MMR, Proteogenomics, PTMs, Mutations,Multi-stage database search.

Poster Presentation : **LIFE.P-230**
Life Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Supported Lipid Bilayer Platform for Macromolecular Detection Applications

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Chemical Engineering, Sungkyunkwan University, Korea

The supported lipid bilayer (SLB) platform is a versatile biomimetic lipid membrane that is widely used in chemical and biological sensing applications. To date, it has proven challenging to fabricate highly biomimetic SLBs with existing methods, e.g., vesicle fusion, because they only work with a limited range of lipid compositions and solid supports. In particular, there is growing interest to develop SLBs that contain high cholesterol fractions due to enhanced biomimetic character and durability. In this work, we developed a highly efficient protocol called the solvent-assisted lipid bilayer (SALB) method to fabricate high-quality SLBs. The SALB method allows cholesterol-rich SLBs to be prepared with tunable cholesterol fractions up to ~52 mol%. As an application example, we demonstrated that fatty acids and monoglyceride derivatives induce distinct membrane morphological responses in SLBs, as indicated by quartz crystal microbalance-dissipation (QCM-D) measurements. While fatty acid addition to SLBs induced tubule formation with a greater extent of membrane remodeling at higher cholesterol fractions, monoglyceride addition caused bud formation with a lower degree of membrane remodeling at higher cholesterol fractions. Altogether, our findings demonstrate how SLBs can function as highly sensitive detection platforms based on triggering specific membrane morphological responses and such capabilities along with other advantageous properties of SLB platforms can be useful for a wide range of medical and biotechnology applications such as cancer diagnostics.

Poster Presentation : **ORGN.P-231**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Enhanced thermoelectric performance of SWNT/organic small molecule (OSM) hybrid materials by tuning the electronic structure of OSMs

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

The thermoelectric (TE) effect is one of the most appealing concepts for renewable energy conversion techniques as they immediately recover disused heat to utilizable electrical power by harnessing temperature gradient. In this regard, numerous studies on inorganic semiconductor-based TE materials witnessed remarkable ZT (figure of merit) values over 1.0, highlighting their commercially available power conversion efficiency. However, their salient features such as intrinsically high thermal conductivities (κ), toxicity, rarity, and brittleness evoked the necessity of organic-inorganic hybrid materials which can reduce κ value by impeding phonon transport, but also can grant flexibility to as-fabricated devices. Among various organic-inorganic composites, nanostructured single-walled carbon nanotube/organic small molecule (SWNT/OSM) hybrid materials have drawn significant attention as an alternative source for renewable energy, as they possess high Seebeck coefficients as well as low κ originated from OSMs. It was assumed that power factors can be increased by modulating the electronic structure of OSMs within nanocomposites, provided that the Seebeck coefficient-electrical conductivity correlation could be meticulously controlled. Until now, only a few SWNT/OSM-based TE materials have been investigated to increase the Seebeck coefficient and power factor by systematically tuning the individual electronic level of OSMs. Herein, we synthesized three π-conjugated small molecules; PBBT (as a control), mPBBT, and dmPBBT. The highest occupied molecular orbital (HOMO) levels and band gaps (Eg) of mPBBT and dmPBBT were controlled by introducing one and two electron-donating groups onto the π-conjugated backbone, respectively. Our study revealed that the Seebeck coefficient and power factor can be improved by fine-tuning the HOMO level and the band gap of OSMs. This is an excellent example of enhancing thermoelectric performance by controlling the electronic structure of OSMs.

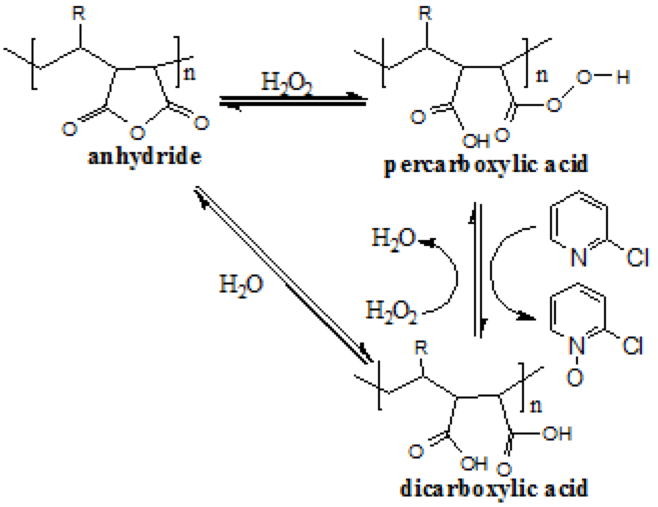
Poster Presentation : **ORGN.P-232**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Recyclable Anhydride Catalyst for H2O2 Oxidation : N-oxidation of Pyridine Derivatives

Sang Hee Lee[*], Dong Hee Kim, Ghellyn Gajeles, Se Mi Kim

Department of Chemistry, Kunsan National University, Korea

Recyclable Anhydride Catalyst for H2O2 Oxidation : N-oxidation of Pyridine DerivativesGhellyn Gajeles, Dong Hee Kim, Se Mi Kim, Sang Hee Lee*Department of Chemistry, Kunsan National University, KoreaPeroxycaroxylic acids(POCA) such as mcpba are useful oxidant and are formed from H2O2 and carboxylic anhydride in situ. Thus, carboxylic anhydride-H2O2 oxidation system can oxidize various organic compounds in the absence of any other catalyst. Generally, equivalent amount of anhydride is required and not reusable. Here, we evaluated anhydride containing polymers as a reusable catalyst in H2O2 oxidation. Fast reaction of anhydride and H2O2 give POCA. After oxidation reaction, resulted dicarboxylic acid in polymer is converted to anhydride spontaneously. The catalytic activity of the polymer come from the regeneration of anhydride during H2O2 oxidation reaction. In addition, the polymer is easily recovered and reused without any treatment because the polymer catalyst is totally not soluble in water. The scope of the oxidation will be described.



Poster Presentation : **ORGN.P-233**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Highly Efficient One-Pot Synthesis of Coumarins from Ynamides and Salicyladehydes

Huen Ji Yoo, So Won Youn*

Department of Chemistry, Hanyang University, Korea

A highly efficient Zn-catalyzed one-pot synthesis of diversely substituted coumarins from ynamides and salicylaldehdyes has been developed. In this process, the sulfonamide moiety of ynamides was successfully recycled, serving as an effective traceless directing group for high regioselectivity in the bond-forming event. This protocol offers straightforward, robust, and sustainable access to a diverse array of valuable coumarins from readily available starting materials with good functional group tolerance, broad substrate scope, and high practicality and efficiency.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-234**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Cu(I)-Catalyzed Divergent Syntheses of Pyrazoles and Pyrroles from *β*-Enamino Esters

Jun Yeong Chang, Su San Jang, So Won Youn*

Department of Chemistry, Hanyang University, Korea

Pyrazoles occupy an important position in medicinal and pesticide chemistry with a wide range of bioactivities. Pyrroles belong to a class of electron-rich heteroaromatic rings, ubiquitous in natural products as well as material sciences. Recently, we have developed Cu(I)-catalyzed oxidative annulations of *β*-enamino esters for the divergent synthesis of two *N*-heterocycles, pyrazoles and pyrroles. It is noteworthy that both processes yielding pyrazoles and pyrroles can tolerate various functional groups. Our experimental findings suggest that both oxidative cyclization reactions implicate radical intermediates generated by SET.

Poster Presentation : **ORGN.P-235**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Borane-catalyzed Nucleophilic Double-Addition of *N*-Heterocycles to Ketones: Synthesis of Bis(heteroaryl)compounds with All-Carbon Quaternary Center

Seunghoon Kook, Yunmi Lee*

Department of Chemistry, Yonsei University, Korea

Indole derivatives are well-known to have numerous biological properties and are used as antibiotics in pharmaceutical industry. Among the indole derivatives, bis(indolyl)structures are recognized to be the core structure of natural products and pharmaceuticals. In this report, we describe a borane-catalyzed nucleophilic double-additions of *N*-heterocycles to ketones; employing diverse ketones ranging from dialkyl ketones to diaryl ketones with hetereoarenes allowed an efficient synthesis of a variety of bis(indolyl) and bis(pyrrolyl) compounds bearing all-carbon quaternary centers, including tetra-aryl centers. Desired double-addition products were obtained under the mild reaction conditions, releasing H_2O as the only by-product.

Poster Presentation : **ORGN.P-236**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

A benzothiazole-based azo compound as chemosensor for detecting Cu^{2+} and S^{2-} in aqueous media

Seon Min Park, Doo OK Jang*

Department of Chemistry, Yonsei University, Korea

Transition-metal ions have toxic properties, and have harmful effects on the body, causing serious diseases. Copper ion is a prime example of transition-metal ions. Copper ions pose a risk of developing several diseases, if there is an excess in vivo. There is a need to selectively detect and remove copper ions.We have designed and synthesized an azo compound having benzothiazole moiety to optically detect copper ions. The sensor recognized copper ions selectively in aqueous media even in the presence of other metal ions. The resulting Cu-complex detected sulfides with reviving the profile of the azo compound.

Poster Presentation : **ORGN.P-237**

Organic Chemistry

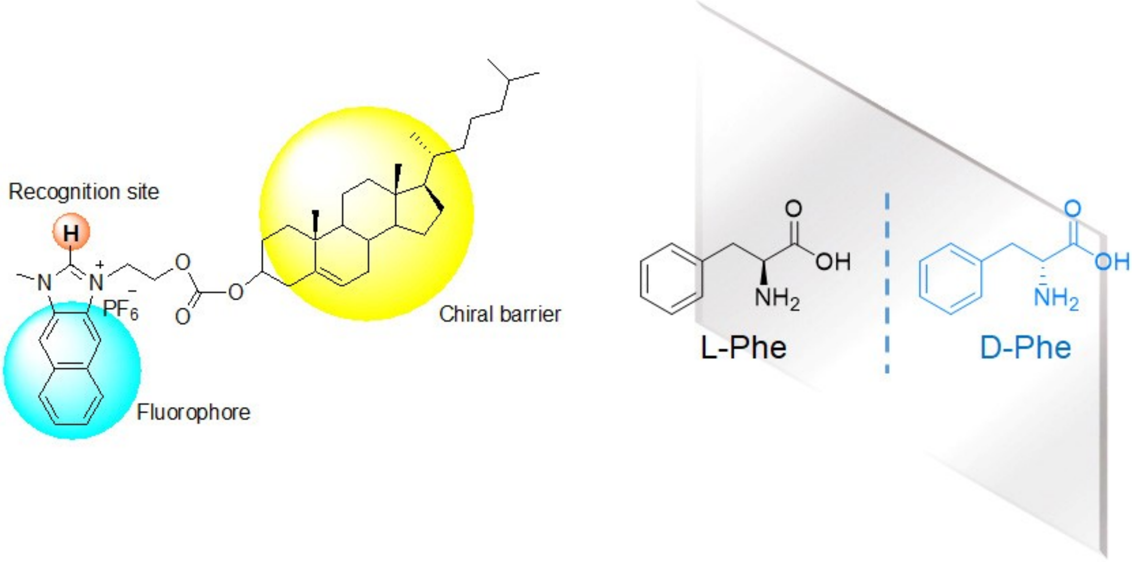
Exhibition Hall 1, FRI 11:00~12:30

A ratiometric fluorescent chemosensor based on naphthoimidazolium-cholesterol derivative for carboxylates chiral recognition

Chaeeon Bae, Songyi Lee*

Department of Chemistry, Pukyong National University, Korea

Fluorescence chemosensors to sense chiral molecules have been actively studied in recent years. In the current study, we report naphthoimidazolium-cholesterol derivative (NI-chol 1) as a fluorescence based chemosensor for chiral recognition, in which naphthoimidazolium serves not only as fluorophore but also as a recognition moiety for anions via imidazolium (C-H)+--anion binding and the cholesterol unit acts as a chiral barrier. In particular, NI-chol 1 displayed unique and distinct ratiometric changes with Boc-D-Phe, on the other hand, Boc-L-Phe induced a negligible change. Furthermore, distinct downfield shift (from 9.64 ppm to 9.96 ppm) of the imidazolium C-H peak were observed for Boc-D-Phe (5 eq.) with severe broadening, which indicates strong ionic hydrogen bonding between the C-H proton and carboxylate.References1 X. Zhang, G.Ko, J. F. Joung, M. Li, Y. Jeong, K. M. K. Swamy, D. Lee, Y. Liu, S. Lee*, S. Park*, T.D. James*, J. Yoon*, Chem. Commun. 2018, 54, 13264-13267.2D. Lee, K. M. K. Swamy, J. Hong, S. Lee*, J. Yoon*, Sens.Actuator B-Chem. 2018, 266, 416-421.


Recognition site
H
N
N
+
PF6
-
O
O
O
Fluorophore
Chiral barrier
O
OH
NH2
L-Phe
O
OH
NH2
D-Phe

Poster Presentation : **ORGN.P-238**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

fluorescent probe-based rhodamine for detection of pH changes in living lysosomal cells

Yongkyun Kim, Songyi Lee*

Department of Chemistry, Pukyong National University, Korea

Intracellular pH helps vital cellular processes, such as endocytosis, cell adhesion, ion transport, and cell growth. Abnormal fluctuation of intracellular pH can cause severe dysfunction, such as indiscriminate cell apoptosis, necrosis, and generation of free radical, and it is associated with serious illness. Thus, Sensing and monitoring of pH changes in live cells are of great importance for understanding of cellular signaling responses. More importantly, the lysosome acts as the cell's recycling center because it performs biologically important events, which include energy metabolism, cell membrane repair, and secretion. Therefore, monitoring changes in lysosomal pH is also essential for understanding lysosome-related diseases and biological processes. In this study, we developed a highly sensitive and selective pH sensor, rhodamine-based fluorescence dye 1. The fluorescent emission of 1 at 588 nm increased with the pH decreasing (from pH 7.0 to 4.0) due to the ring-opening of spirolactam by H+. 1 was used for monitoring pH changes in lysosomes induced by chloroquine, artesunate and dexamethasone. 1 exhibited good water solubility, high quantum yield, as well as fast response to pH changes. our work provides a potential probe 1 for visualizing the intracellular changes of pH in clinical and medical applications.reference : Dayong Lee, K.M.K. Swamy, Joohee Hong, Sensors and Actuators B: Chemical, 2018, 266, 416-421

Poster Presentation : **ORGN.P-239**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Small Triiminopyrrolic Molecular Cage with High Affinity and Selectivity for Fluoride

Hye Jin Han, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A small molecular cage (4) containing three iminopyrrole groups as hydrogen bonding donors has been synthesized on the basis of a hexasubstituted benzene scaffold. ^{1}H and ^{19}F NMR spectroscopic analyses measured in $CDCl_3$ and DMSO provide support for the conclusion that cage 4 binds fluoride with high affinity and complete selectivity to the limit of detection even in the presence of other competing anions, such as chloride, bromide, iodide, and sulfate. Cage 4 was also found to retain the encapsulated fluoride anion within its cavity even after one or two pyrrolic NH protons were subject to deprotonation and in spite of the presumed nitrogen anion-fluoride anion electrostatic repulsion that was expected to result.

Poster Presentation : **ORGN.P-240**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Phenanthroline-Strapped Calix[4]pyrroles as Bicarbonate-Selective Receptors and Anion Binding Affinity Reversal in Highly Polar Solvent System

Nam Jung Heo, **Sung Kuk Kim***

Department of Chemistry, Gyeongsang National University, Korea

Anion receptors **1** and **2** based on calix[4]pyrroles diametrically strapped with a phenanthroline via ester and amide linkages, respectively, have been synthesized. It was revealed by ^1H NMR spectroscopic analysis that receptors **1** and **2** possessing both hydrogen bonding donors and acceptors are able to bind the bicarbonate anion (as its tetraethylammonium (TEA^+) and sodium salts) in $CDCl_3$ as well as highly polar 15% aqueous DMSO with high affinity and selectivity over other anions. Unexpectedly, in less polar $CDCl_3$, receptor **1** having the ester linkages was found to have higher association constants for all test anions than receptor **2** having additional hydrogen bonding donors of the amide groups. In contrast, in even more polar DMSO containing 15% water, the affinity of receptor **2** for anions was significantly enhanced whereas that of receptor 1 drastically decreased with no binding interaction with most anions observed.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-241**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Tripodal receptors for anion and ion pair recognition

Juho Yang, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Tripodal ion pair receptors **1** and **2** consisting of tripyridinylmethyl amine as a cation binding site and indole and urea groups as anion binding motifs have been synthesized. UV/Vis and ^{1}H NMR spectroscopic analysis revealed that both of receptors were capable of binding respective anions and cations as well as ion pairs. In these cases, the cations such as lithium and zinc were bound to the tripodal pyridine units while anions were hydrogen bonded the NHs of the indole amide or urea gro**1** and **2** were significantly enhanced with the cations being complexed with the tripodal pyridinyl group presumably because the cation binding brought the three branches containing urea or amido indole groups in close proximity. As a result, the urea or amido indole groups came to work in a cooperative way to bind anions with higher affinity.

Poster Presentation : **ORGN.P-242**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Dual sensing of the mercury cation using the anthracene appending diazocalix[4]arene

Seung Hyeon Kim, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A anthracene-appending diazocalix[4]arene (1) was synthesized as a fluorescent and chromogenic sensor for cations. UV/Vis and fluorescence spectroscopic analysis revealed that receptor 1 was able to bind specific cations such as calcium, barium, lead and mercury ions displaying different colorimetric and fluorescent signals. Upon the addition of calcium, barium and lead to the solution of the receptor, large red shifts in the maximum absorption peak of receptor 1 took place with remarkable color changes from orange to red. This finding is attributable to the cations bound to the oxygens of phenol units linked to the diazo group of calix[4]arene. By contrast, relatively small color change was observed in the presence of Hg2+ because the cation is bound to the receptor with a different binding mode. 1H NMR spectroscopic analysis confirmed the different binding modes of receptor 1 with mercury relative to other test cations. UV/Vis spectral titration experiments showed that the receptors had the highest affinity for Hg2+ among metal cations (Ka = 8.5*109) tested. By contrast, the fluorescence intensity of receptor 1 is drastically quenched by the complexation with the mercury cation.

Poster Presentation : **ORGN.P-243**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Anion Recognition Features of a Molecular Cage Containing Both Hydrogen Bond Donors and Acceptors

Ju hyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A molecular cage, marcobicycle **1**, containing amide and pyrrole group as hydrogen-bonding donors and imine group as hydrogen-bonding acceptors has been synthesized. Compound **1** was found to recognize tetrahedral oxyanions with high affinities, such as $H_2PO_4^-$, HSO_4^-, SO_4^{2-}, and $HP_2O_7^{3-}$, as well as the spherical halide anions, in chloroform. A single-crystal X-ray diffraction analysis revealed that compound **1** formed 1:1 complex with $H_2PO_4^-$ in the solid state.

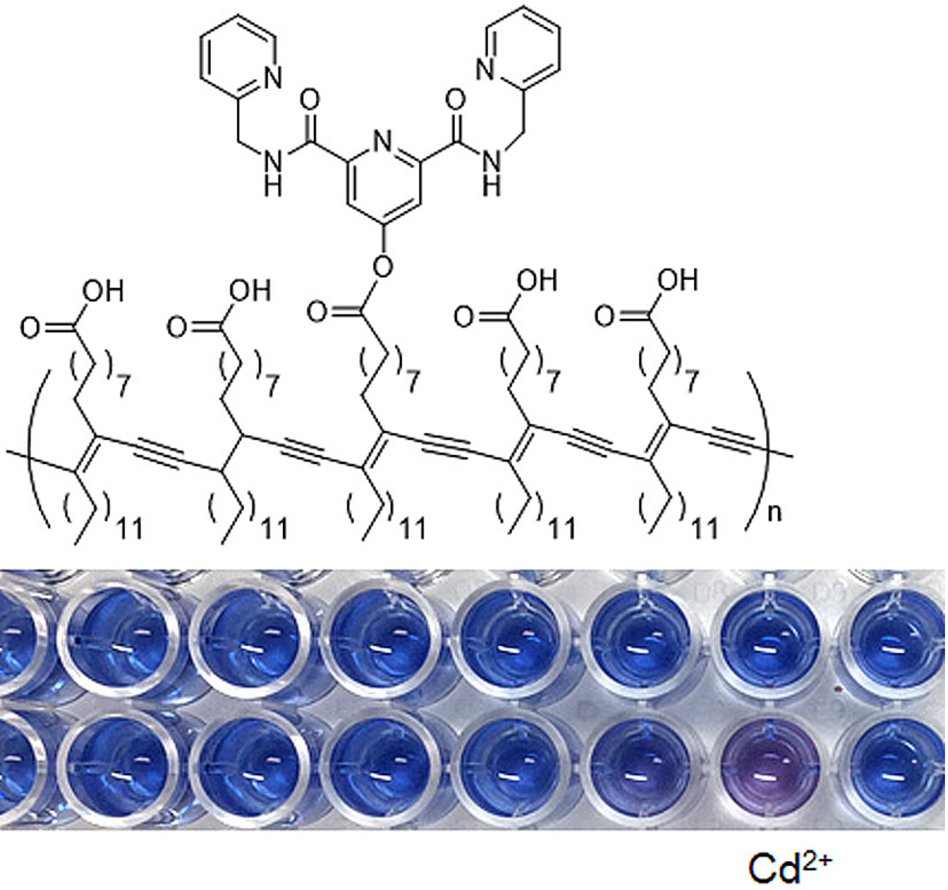
Poster Presentation : **ORGN.P-244**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Dual Colorimetric and Fluorometric Sensor for Cadmium Ion Based on Conjugated Polydiacetylenes

Thanh Chung Pham, Songyi Lee*

Department of Chemistry, Pukyong National University, Korea

In recent years, pollution associated with the presence of heavy metal ions in the environment has been extensively investigated. Among the various heavy metal ions, cadmium (Ⅱ), is one of the most hazardous and carcinogenic metals, because of its widespread use in fields such as metal alloys, electroplating, stains, fertilizers, as well as in rechargeable batteries. As a result, a number of analytical techniques have been developed to detect Cd^{2+}. However, the application of these methods is restricted due to the complexity of sample preparation and instrumentation. Therefore, a rapid and convenient detection method for Cd^{2+} is imperative. In this regard, we present our findings involving the development of a simple and cost-effective sensor for naked-eye detection of Cd^{2+} that does not require an external power source.Polydiacetylenes (PDAs) have received increasing attention as smart materials owing to their unique properties.[1-3] Upon addition of various stimuli, the blue PDAs can undergo a colorimetric transition from blue to red along with a change from non-fluorescent to fluorescent. The optical changes can be readily detected using the naked eye and by absorption and fluorescence spectrometers. These properties make PDAs excellent materials for use in platforms for sensing chemical or biological targets. References1. Chen, X.; Zhou, G.; Peng, X.; Yoon, J. Chem. Soc. Rev. 2012, 41, 4610-4630.2. Lee, S.; Kim. J. -Y.; Chen, X.; Yoon, J. Chem. Commun. 2016, 52, 9178-9196.3. Lee, S.; Lee, J.; Lee, M.; Cho, Y. K.; Baek, J.; Kim, J.; Park, S.; Kim, M. H.; Chang, R.; Yoon, J. Adv. Funct. Mater. 2014, 24, 3699-3705.


Cd^{2+}

Poster Presentation : **ORGN.P-245**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Design of donor material containing fluorinated benzothiadiazole unit for increasing of power conversion efficiency

Shimiao Zhang, **Hongsuk Suh**[1,*]

PUSAN NATIONAL UNIVERSITY, China
[1]*Department of Chemistry, Pusan National University, Korea*

During the past few decades, polymer solar cells (PSCs) have drawn great interest as one of the potential alternative technologies for utilizing the renewable solar energy, because of their advantages such as lightweight, low cost, large-areas and flexible solar modules through roll-to-roll processing. In order to obtain high-performance PSCs, a polymer containing fluorinated dithienylbenzothiadiazole (DTBT) as an electron accepting group and 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole as an electron donating group were successfully synthesized. Due to the strong electron-withdrawing ability of fluorine, we introduced fluorine atom into the conjugated polymer to improve the efficiency of organic solar cells, and the synthesized polymer having fluorine atoms indicated deep highest occupied molecular orbital energy levels. A power conversion efficiency (PCE) of 3.17% was achieved in the device by using **PTTIF2**:PCBM (1:1w/w) blend without additive, and a PCE of 4.36% was achieved in the device by using **PTTIF2**:PCBM (1:1w/w) blend with chloronaphthalene (CN) additive.

Poster Presentation : **ORGN.P-246**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Design of pyrimidine-based polymers consist of thiazolo[5,4-*b*]pyridine as electron-deficient unit applied to the polymer solar cells

Shimiao Zhang, Hongsuk Suh[1,*], Juwon Kim[2]

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

Environment problems such as pollution caused by making energy have been recognized as one of the most serious problems. Polymer solar cell (PSC) using solar energy generation is eco-friendly and renewable energy because of their advantages. It doesn’t have a polluted smoke and also has low cost, light-weight, easy to flexibility and processing. We synthesized π-conjugated polymers based on pyridine to use for PSC including electron-withdrawing groups (EWG), 2-{3-[4,6-bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-*b*]pyridine (**mTP**), and confirmed the properties of position of functional group. π-conjugated polymers, **mPTPBDT-EH**, **mPTPBDTT-EH** and **mPTPTTI**, were based on 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole (TTI), or benzo[1,2-*b*;3,4-*b*']dithiophene (BDT), or 4,8-bis(5-thiophen-2-yl)benzo[1,2-*b*:4,5-*b*']dithiophene (BDTT) as electron rich groups and mTP as EWG. The device including **mPTPTTI** showed a V_{OC} of 0.72 V, a J_{SC} of 4.95 mA/cm^2, and a *FF* of 0.32, giving a PCE of 1.15%.

Poster Presentation : **ORGN.P-247**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Characteristics of thiazolo[5,4-*b*]pyridine as electron-withdrawing units in the PSCs

Shimiao Zhang, Hongsuk Suh[1,*]

PUSAN NATIONAL UNIVERSITY, China
[1]*Department of Chemistry, Pusan National University, Korea*

Polymer solar cells (PSCs) are engaging attention as a solution to the coming global energy problem in terms of converting solar power into electrical energy. Compared to various types of solar cells, PSCs has great potential because of their mechanical flexibility and various synthesis routes.[1] Polymers (**pPTPBDTT-EH, pPTPTTI, pPTPBDT-EH**) which were composed of 4,8-bis(5-thiophen-2-yl)benzo[1,2-*b*:4,5-*b*']dithiophene (BDTT), or 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole (TTI), or benzo[1,2-*b*;3,4-*b*']dithiophene (BDT), as electron-donating parts and 2-{4-[4,6-bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-*b*]pyridine (pPTP) as electron-accepting parts, were made. Herein, pPTP is a newly devised material for the reason of a novel electron-deficient group in the cells and situated at the para position of the pyrimidine backbone. In the devised polymers, **pPTPTTI** showed the highest efficiency. The cell was composed of **pPTPTTI** and $PC_{71}BM$ (1:1) with 3% CN additive indicated a fill factor of 0.31, a J_{SC} of 4.41 mA/cm^2, a V_{OC} of 0.83 V, showing a power conversion efficiency of 1.13%.[1] Su, Y.-W; Lan, S.-C.; Wei, K.-H. *Organic photovoltaics. Mater. Today*, **2012**, *15*, 554-562.

Poster Presentation : **ORGN.P-248**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of conjugated random copolymers consisting bithiophene-dicarboximide and thienyl-thieno-indole for improving performance for organic solar cells

Lingxin Meng, Hongsuk Suh[1,*]

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

Polymer solar cells (PSCs) have received wide interests and have developed quickly in recent years because of its advantages of low cost, large area, ultra-weight and solution processing in comparison with the traditional silicon-based solar cells. In this work, we designed and synthesized random copolymers as donor which are based on BTI and TTI units with different ratios. The 2,2’-bithiophene-3,3’-dicarboximide(BTI) unit has two carbonyl groups conjugated with the thiophene units for the generation of electron-withdrawing ability, one nitrogen atom for the introduction of alkyl side chain to improve the solubility. 6-(2-Thienyl)-4*H*-thieno[3,2-*b*]indole (TTI) has five membered thiophene ring substituted the six membered benzene ring of the carbazole. We ever used TTI in PSCs for improving the charge carrier induced to generate more efficient electron-donating ability. We synthesized conjugated random copolymers, **P0, PBTI7, PBTI5** and **PBTI3** containing BTI as the electron-deficient unit and TTI as the electron-rich unit. The **PBTI3** with the highest amount of TTI unit displayed the highest molar absorption coefficient and mobility. The device based on **PBTI3**:$PC_{71}BM$ showed the best performance with a V_{OC} of 0.72 V, a J_{SC} of 6.78 mA/cm^2, and a FF of 0.54, giving a PCE of 2.64%.

Poster Presentation : **ORGN.P-249**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Syntheses of Conjugated Polymers Containing Carbazole derivate as a Donor in PSCs

Lingxin Meng, Hongsuk Suh[1,*]

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

Polymer solar cells have increasing attention due to their advantages such as lightweight, low cost, flexibility. Moreover, it can be applied to a roll-to-roll printing process, which is good for mass-production.[1] In this study, we synthesized carbazole-based conjugated polymers and introduced as donor material of active layer. By using Suzuki polymerization, **HS-5610, HS-5613** and **HS-5614** are synthesized. Synthesized donor-acceptor (D-A) polymers have carbazole derivate as electron-donating unit. Also, electron-accepting units are thieno[3,4-*c*]pyrrole-4,6-dione (TPD), isoindigo (ID) and alkyl-2,20-bithiophene-3,30-dicarboximide (BTI) units for each polymers. The device introducing **HS-5614** indicated a PCE of 0.41% with a V_{OC} of 0.65 V, a J_{SC} of 2.04 mA/cm^2, and a FF of 31.2%. These results manifested that synthesized D-A polymers have significance to act as donor materials of active layer.[1] Su, Y.-W; Lan, S.-C.; Wei, K.-H. *Organic photovoltaics. Mater. Today*, **2012**, *15*, 554-562.

Poster Presentation : **ORGN.P-250**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Isoindigo-based Conjugated Polymers Consisting of 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole (TTI) for the Improvement of Performance of Organic Solar Cells

Lingxin Meng, Hongsuk Suh[1,*]

Pusan National University, Korea

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

Organic Solar Cells (OSCs) are promising alternatives of solar-cell in terms of energy generation due to their abundance of constituent elements and base materials, low cost, and relatively easy to synthesis.[1]In this research, 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole (TTI) and isoindigo (ID) were used for conjugated polymers. Alternating and random copolymers including TTI and ID units were designed. From the UV-vis absorption spectra of the random copolymers, significant red shift from the maximum peaks and a broader full width at half maximum (fwhm) with higher ID unit ratio were observed. Conjugated polymers exhibit lower gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels with increased percentage of ID as electron accepting groups. The device composed of **PTTIID-7** and PCBM (1:2) had shown V_{OC}, J_{SC} and fill factor (*FF*) value of 0.63 V, 12.3 mA/cm^2, and 0.52 respectively which gives the PCE of 4.03%.[1] Su, Y.-W; Lan, S.-C.; Wei, K.-H. *Organic photovoltaics. Mater. Today*, **2012**, *15*, 554-562.

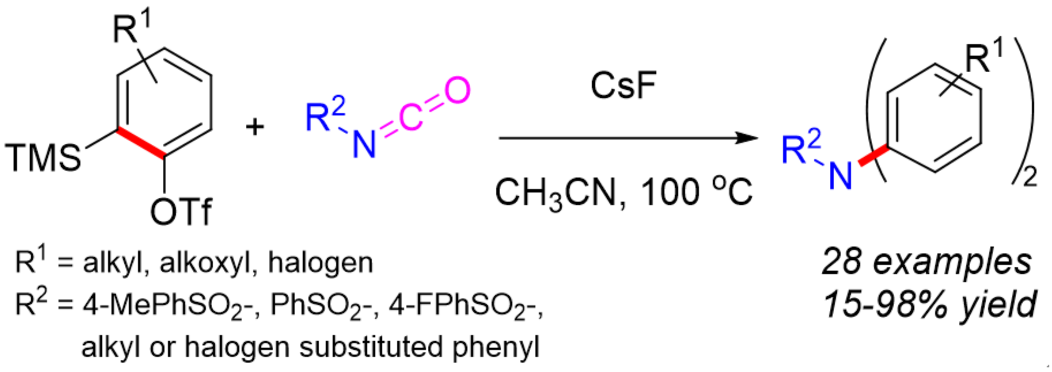
Poster Presentation : **ORGN.P-251**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Transition-Metal-Free Diarylation of Isocyanates with Arynes

Woo Cheol Jang, Haye Min Ko[1,*]

Department of Bio-nano chemistry, Wonkwang University, Korea
[1]*Department of Bio-nanochemistry, Wonkwang University, Korea*

A facile method for the transition-metal-free diarylation of isocyanates with arynes in the presence of cesium fluoride has been developed, which affords functionalized diaryl amines in moderate to excellent yields. This reaction has good functional group tolerance and provides excellent regioselectivity by utilizing a methoxy-substituted aryne precursor.



Poster Presentation : **ORGN.P-252**

Organic Chemistry

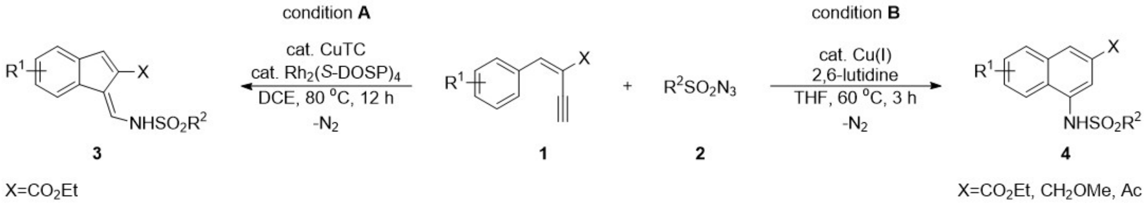
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Benzofulvenes or Naphthalenes through Transition Metal-Catalyzed Transannulation of Enynyl Triazoles

Kiun Cheong, Ji Kwon Lee, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

(A) Rhodium-catalyzed denitrogenative cyclization of (E)-ethyl 2-(1-alkyl and arylsulfonyl-1H-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 developed for the synthesis of a large number of functionalized benzofulvenes. Moreover, the synthesis of benzofulvenes was demonstrated as a one-pot method through tandem copper-catalyzed [3 + 2] cycloaddition and rhodium-catalyzed denitrogenative cyclization from (E)-ethyl 2-benzylidenebut-3-ynoates and N-sulfonyl azides.(B) A synthetic method for ethyl 4-(alkyl or arylsulfonamido)-2-naphthoates from ethyl (E)-α-ethynyl-β-aryl- α,β-unsaturated esters (1) and N-sulfonyl azides (2) in the presence of 2,6-lutidine in THF at 60 oC for 3 h was developed in one step, in which a copper(I)-catalyzed 1,3-dipolar cycloaddition, ketenimine formation, and 6π-electrocyclization followed by [1,3]-H shift tandem reaction took place. This method enabled efficient synthesis of a wide range of 1-aminonaphthalene and 3-aminobenzofuran and 3-aminobenzothiophene derivatives with the release of molecular nitrogen.



Poster Presentation : **ORGN.P-253**

Organic Chemistry

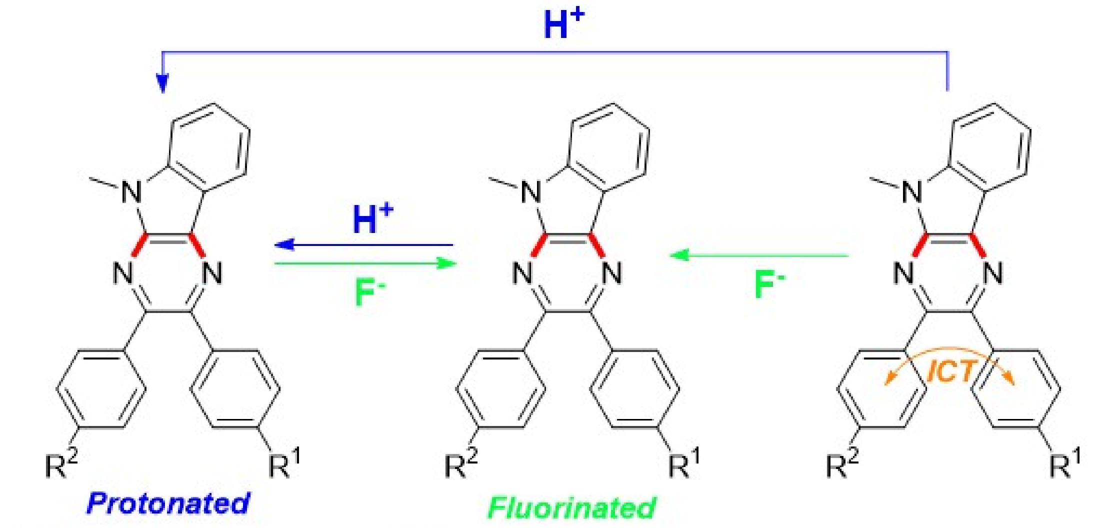
Exhibition Hall 1, FRI 11:00~12:30

Pyrazinoindole-Based Lewis-Acid/Base Assembly through Intriguing Intramolecular Charge-Transfer Switching from the Dual-Sensing of Acid and Fluoride

Seong Bin Jang, Kiun Cheong, Chanyoung Maeng, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Pyrazinoindole-based Lewis-acid/base assemblies are prepared through the use of regioselective formal [3 + 3] cycloaddition reactions and their intriguing photophysical properties are described. The assemblies exhibit strong emissions in THF solution, which are attributed to through-space intramolecular charge-transfer (ICT) transitions between the branched Lewisacid/ base moieties. Furthermore, these show ratiometrically color-change responses in PL titration experiments, which give rise to new colors through turn-on emissions ascribable to ICT transitions that alternate between the pyrazinoindole units and each triarylboryl or amino moiety, a consequence of the binding of the fluoride or acid. Pieces of filter paper covered by these assemblies demonstrated exhibited blue-shifted color changes when immersed in aqueous acidic solutions, suggesting that these are promising candidate indicators that detect acid through emissive color. Computational data for these assemblies and their corresponding adducts verify the existence of ICT transitions that alternate through fluoride or acid binding.



R^1 = $B(Mes)_2$, R^2 = $NHEt_2^{\oplus}$
[**PI1**•H]

R^1 = $NHEt_2^{\oplus}$, R^2 = $B(Mes)_2$
[**PI2**•H]

R^1 = $BF(Mes)_2^{\ominus}$, R^2 = NEt_2
[**PI1**•F]

R^1 = NEt_2, R^2 = $BF(Mes)_2^{\ominus}$
[**PI2**•F]

R^1 = $B(Mes)_2$, R^2 = NEt_2, **PI1**

R^1 = NEt_2, R^2 = $B(Mes)_2$, **PI2**

- ***Color-changed & turn-on emission by ion sensing***
- ***Controlled ICT***
- ***Fully reversible process***
- ***Acid indicator***
- ***Regioselective synthesis***

Poster Presentation : **ORGN.P-254**

Organic Chemistry

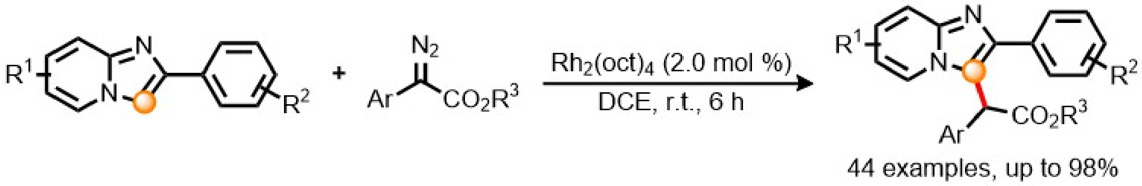
Exhibition Hall 1, FRI 11:00~12:30

Rh-Catalyzed Regioselective C3-Alkylation of 2-Arylimidazo[1,2-a]pyridines with Aryl Diazoesters

Hyeonsik Eom, Seong Bin Jang, Sang Hoon Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Imidazo[1,2-a]pyridines are significant privileged scaf-folds in azaheterocycle chemistry,[1] and they are commonly found in natural products, pharmaceuticals, and biologically active compounds. Among azaheterocycles, imidazopyridines and espe-cially 3-alkyl-2-arylimidazo[1,2-a]pyridines are not only essential pharmacophores but also practical synthetic intermediates that can be easily converted into valuable molecules.A regioselective C3-alkylation based on the reaction of 2-arylimidazo[1,2-a]pyridines with a wide range of aryl α-diazoesters in the presence of a Rh(II) catalyst in dichloroethane at room temperature was developed. This method could be applied in the synthesis of benzoimidazoquinolizinone and cyclo-heptaimidazopyridinone, which are novel heterocyclic scaffolds.



Poster Presentation : **ORGN.P-255**

Organic Chemistry

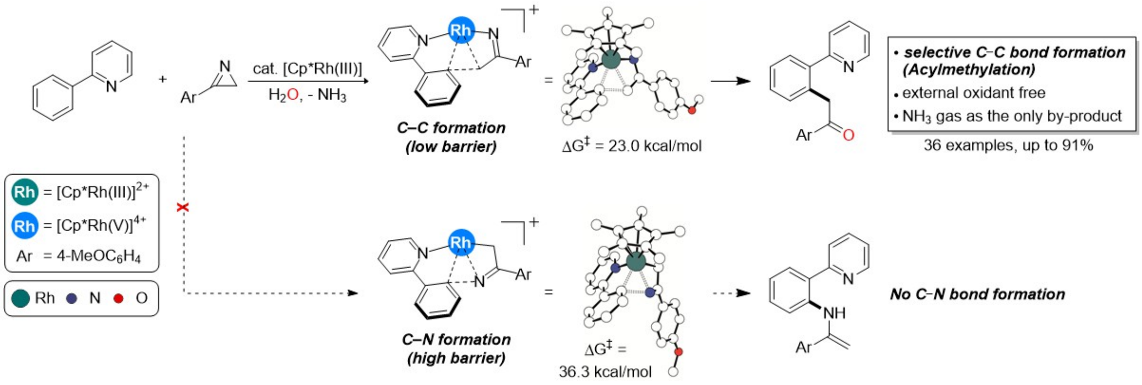
Exhibition Hall 1, FRI 11:00~12:30

Selective C–C bond formation through Rh-catalyzed C–H activation reaction of 2-arylpyridines with 3-aryl-2H-azirines

Ji Kwon Lee, Hyeonsik Eom, Mu-Hyun Baik[1,*], Phil Ho Lee[*]

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

A novel method for the synthesis of acylmethyl-substituted 2-arylpyridine derivatives using 3-aryl-2H-azirines was developed by exploring a prototype reaction using DFT-calculations and carrying out targeted experiments guided by the calculated mechanism. 2H-Azirine was initially hypothesized to ring-open at the metal center to furnish familiar metal nitrene complexes that may undergo C–N coupling. Computational studies quickly revealed and prototype experimental work confirmed that neither the formation of the expected metal nitrene complexes nor the C–N coupling were viable. Instead, azirine ring-opening followed by C–C coupling was found to be much more favorable to give imines that readily underwent hydrolysis in aqueous conditions to form acylmethyl-substituted products. This new method was highly versatile and selective toward a wide range of substrates with high functional group tolerance. The utility of the new method is demonstrated by a convenient one-pot synthesis of biologically relevant heterocycles such as pyridoisoindole and pyridoisoqunolinone.



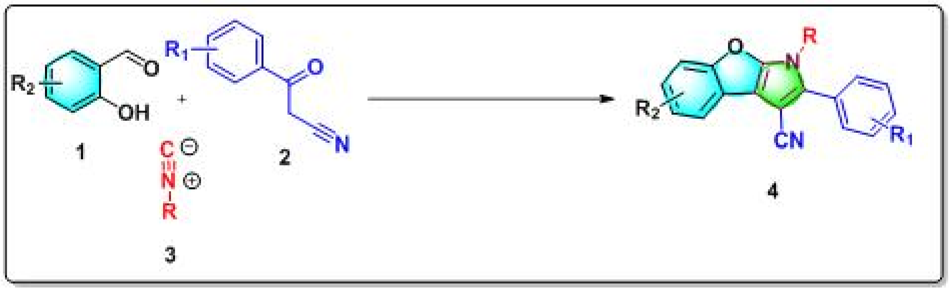
Poster Presentation : **ORGN.P-256**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Brønsted Acid-Promoted One-pot Synthesis of Tricyclic Benzofuro[2,3-b]pyrroles Utilizing Reactive Nitrilium Trapping Approach

Sandip gangadhar Balwe, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

The first Bronsted acid-catalyzed highly efficient one-pot cascade reaction for the synthesis of new nitrogen-fused tricyclic benzofuro[2,3-b]pyrroles has been discovered. The reaction sequence involves a Knoevenagel condensation of a 2-hydroxybenzaldehydes with aroylacetonitrile followed by subsequent nucleophilic addition of the divalent isocyano carbon to generate highly reactive nitrilium carbon, which could readily trapped by an adjacent phenolic group of 2-hydroxybenzaldehydes to access diverse benzofuro[2,3-b]pyrrole derivatives in one-step.



Poster Presentation : **ORGN.P-257**

Organic Chemistry

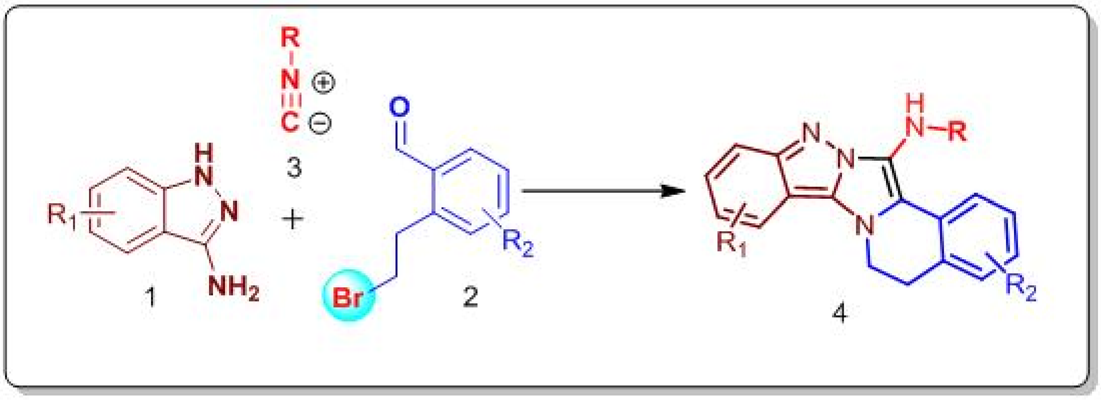
Exhibition Hall 1, FRI 11:00~12:30

A Metal-free Synthesis of nitrogen fused Polycyclic Dihydroisoquinolinium (DHIQ) derivatives: One-pot Double-Annulation Cascade

Sandip gangadhar Balwe, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

A highly reactive cyclic iminium ion induced one-pot double annulation cascade for the synthesis of nitrogen fused polycyclic dihydroisoquinolinium derivatives has been presented. The main key features of this one-pot cascade are metal-free approach, robust protocol, mild reaction conditions, operational simplicity and one-step construction of new privileged polyheterocycles.



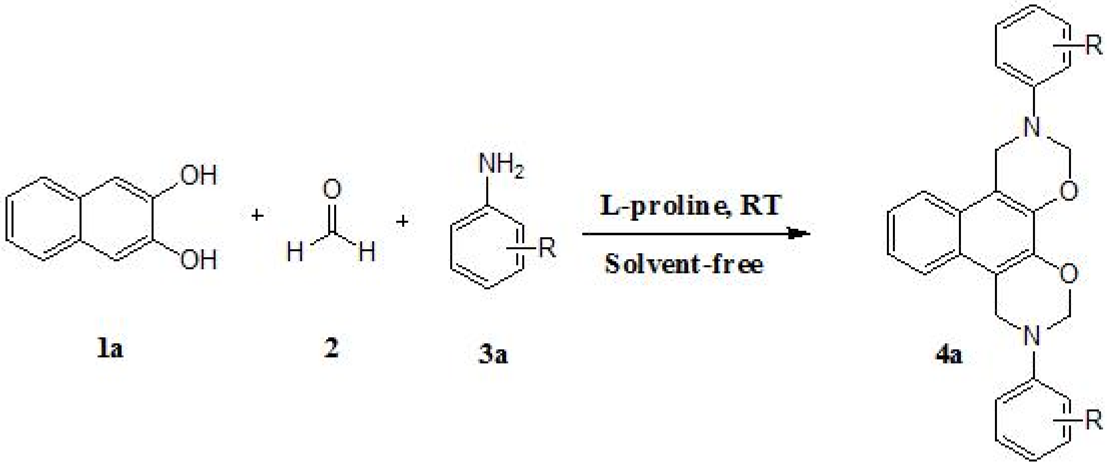
Poster Presentation : **ORGN.P-258**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

L-proline catalyzed highly efficient and green method for the synthesis of novel naphtho-bis[1,3]oxazine derivatives under solvent-free conditions

Amol Jadhav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

An efficient and eco-friendly procedure for the synthesis of novel 3,10-diphenyl-2,3,4,9,10,11-hexahydronaphtho[1,2-e:4,3-e']bis[1,3]oxazine derivatives has been developed through a one-pot three-component condensation of 2,3-dihydroxynaphthalene, formaldehyde, and anilines, in the presence of catalytic amount of L-proline as a catalyst under solvent-free conditions at ambient temperature. This new procedure offers several advantages such as shorter reaction times, excellent yields, a wide range of functional group tolerance, easy experimental work-up procedure and column chromatography-free method. This procedure useful for the synthesis of heterocyclic compounds.



Poster Presentation : **ORGN.P-259**

Organic Chemistry

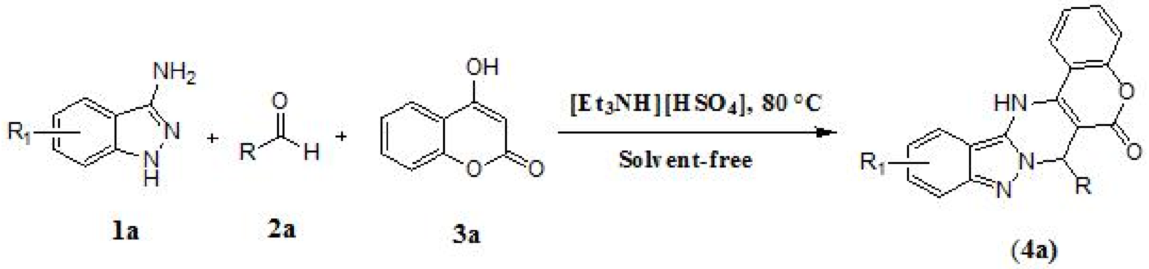
Exhibition Hall 1, FRI 11:00~12:30

One-pot three-component synthesis of novel chromeno pyrimido[1,2-b]indazolone derivatives using ionic liquid as a reusable catalyst under solvent-free conditions

Amol Jadhav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

An efficient one-pot synthesis of novel chromeno pyrimido[1,2-b]indazolone derivatives via three-component condensation reaction of 1H-indazol-3-amine, aldehydes and 4-hydroxycoumarin in the presence of Bronsted acidic ionic liquid [Et3NH][HSO4] as a catalyst under solvent-free reaction conditions is presented. This ecofriendly protocol offers several advantages such as a cost effective procedure with excellent yields, short reaction time, simple workup, recovery and reusability of catalyst with broad scope of usable substrates, column chromatography-free method. This has made the protocol sustainable and economic.



Poster Presentation : **ORGN.P-260**

Organic Chemistry

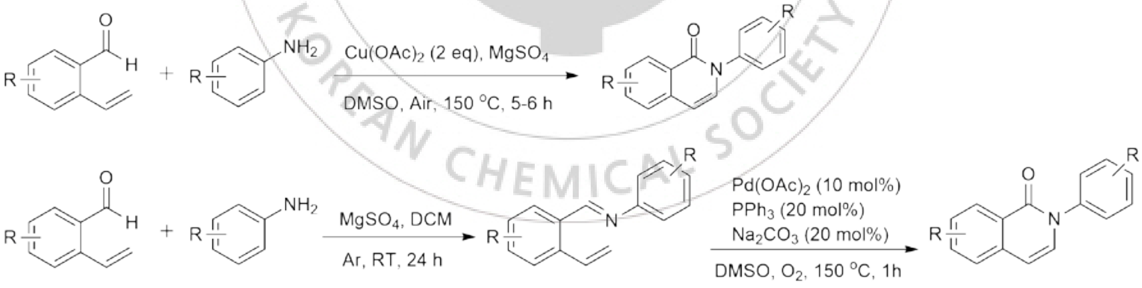
Exhibition Hall 1, FRI 11:00~12:30

Aerobic Oxidative Cyclization Approaches to 2-Phenylisoquinolin-1(2H)-one

Jiyeon Lee, Hun Young Kim[1,*], Kyungsoo Oh[1,*]

Chung-Ang University, Korea
[1]*College of Pharmacy, Chung-Ang University, Korea*

Isoquinolin-1(2H)-ones, one of the nitrogen-containing heterocycles, are important structural components present in numerous potent drugs and biologically active natural products. The development of new methods for the synthesis of isoquinolin-1(2H)-ones is an important topic in chemical research. Herein, we present inter- and intra-molecular aerobic aza-cyclization reactions to 2-phenylisoquinolin-1(2H)-ones under two different catalytic systems using palladium and cooper metals.



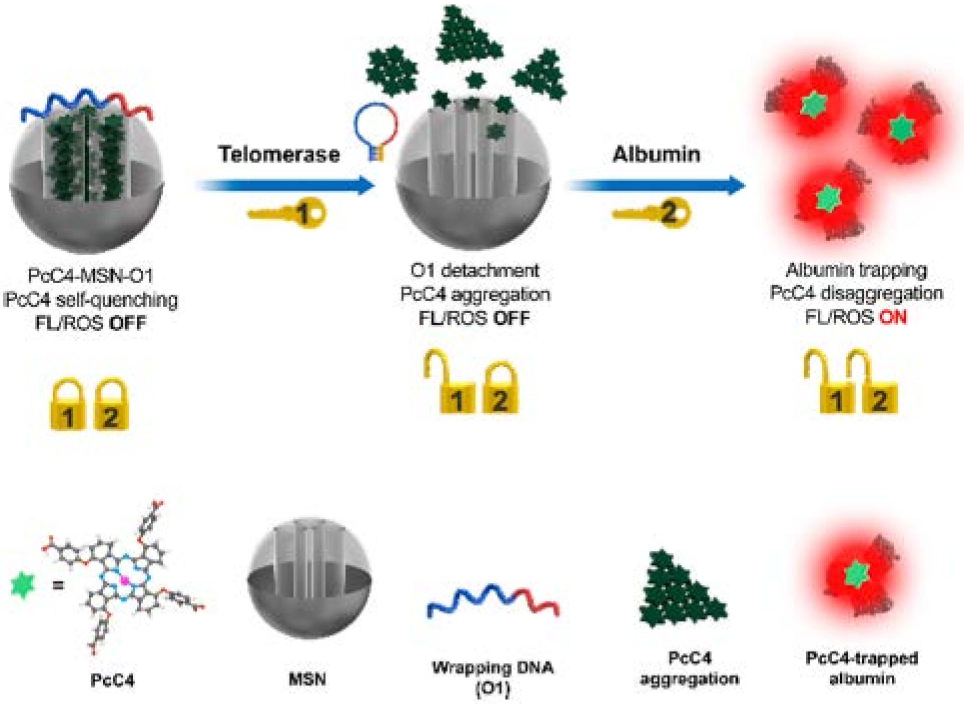
Poster Presentation : **ORGN.P-261**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Strategy to develop tumor homing therapy utilizing protein sequence responsive nanophotosensitizer complex

Jeewon Chung, Xingshu Li[1], Nahyun Kwon, Juyoung Yoon*

Department of Chemistry and Nanosciences, Ewha Womans University, Korea
[1]*College of Chemistry, Fuzhou University, China*

Recent studies focus on developing activatable photosensitizers (aPS) which are only reactive to tumor related stimuli, in order to accurately target tumor cells. This paper introduces a protein sequence reactive aPS(PcC4-MSN-O1) and it only turns on by two specific protein targets. PcC4 is self-quenched in the structure of PcC4-MSNO1, however, the photoactivity is turned on when it reacts with telomerase and albumin in order. This indicates that PcC4-MSN-O1 has clear photoactivity in cancer cells compared to normal cells. Moreover, when tested with xenograft bearing mice model, PcC4-MSN-O1 was accumulated in the HeLa tumor cells and also tumor growth was obviously inhibited after laser irradiation. Finally, the time-regulated activation and quick excretion from the body was checked. Therefore, PcC4-MSN-O1 is expected to be a good solution to minimize the photodynamic therapy (PDT) side effects.


PcC4-MSN-O1
PcC4 self-quenching
FL/ROS OFF
Telomerase
1
O1 detachment
PcC4 aggregation
FL/ROS OFF
Albumin
2
Albumin trapping
PcC4 disaggregation
FL/ROS ON
1 2
1 2
1 2
=
PcC4
MSN
Wrapping DNA (O1)
PcC4 aggregation
PcC4-trapped albumin

Poster Presentation : **ORGN.P-262**

Organic Chemistry

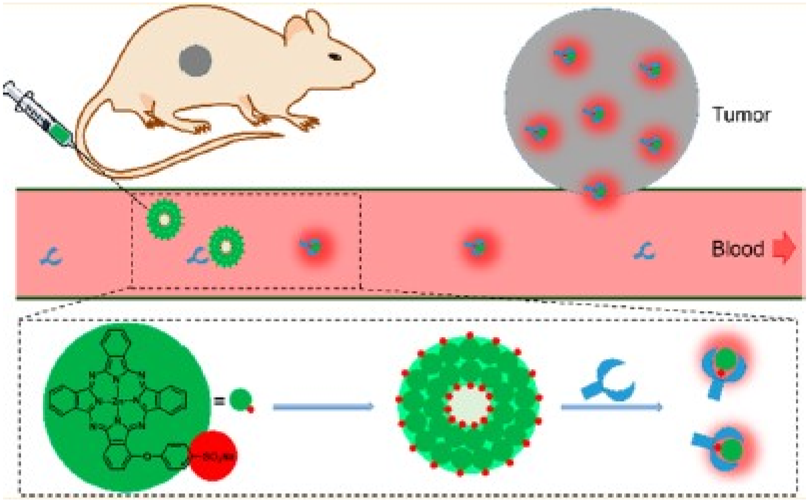
Exhibition Hall 1, FRI 11:00~12:30

A One-for-all Switchable Nanotheranostics: Photosensitizer Detecting Albumin *In Vivo* From the Disassembly of Nanovesicles

Dayeh Kim, Xingshu Li[1], Nahyun Kwon, Sun Choi[2,*], Juyoung Yoon[*]

Department of Chemistry and Nanosciences, Ewha Womans University, Korea
[1]*Fuzhou University, China, China*
[2]*College of Pharmacy, Ewha Womans University, Korea*

Theranostics that can indicate the expression of biomarkers and simultaneously transport therapeutic agents play a key role in basic biological studies as well as in treatment applications. Among many biomarkers, Albumin is one of the most promising candidates for potential disease diagnostics and it is used as a drug delivery carrier for many years. However, there are only few cases showing the specific interactions of exogenous probes with albumin *in vivo*, and slow fabrication processes and potential toxicity of the complexes were main problems of nanocompound delivery systems. In this study, we demonstrate a simplistic switchable nanotheranositc (NanoPcS) for both albumin detection and cancer treatment. Especially, the disassembly of injected NanoPcS causes the in vivo specific binding between albumin and PcS, and the binding is confirmed using an inducible transgenic mouse system. According to the results of fluorescence imaging and antitumor tests on different tumor models, NanoPcS has higher-level tumor-targeting ability and the potential for time-modulated, activatable photodynamic therapy (PDT).


Tumor
Blood

Poster Presentation : **ORGN.P-263**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Turn-on fluorescent probe for the selective detection of ATP in mitochondria and lysosomes

Gain Baek, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The importance of ATP is well-known because it is an essential energy source in all living things. Besides, low levels of ATP are indicators of cardiovascular disease, Parkinson’s disease, disease and ischemia. So, since now, many research groups have developed various kinds of ATP detecting probes. In this study, we demonstrate fluorescent “turn-on” probe based on rhodamine derivatives, bearing thiourea groups, for the detection of adenosine-5′-triphosphate (ATP) through hydrogen bond interactions. Probes shows obvious color and fluorescence change with the presence of ATP. Moreover, these probes can be used to image ATP in HeLa cells. Probe 2 and 5 were found to locate in mitochondrial ATP in HeLa cells. On the other hand, probe 4, bearing morpholine group, was mainly located to lysosomes

Poster Presentation : **ORGN.P-264**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Albumin dimers binding phthalocyanine photosensitizers: green and efficient way enhancing PDT efficacy

Seon Ye Heo, Xingshu Li[1], Nahyun Kwon, Jian-Dong Huangb*[1,*], Sun Choi[2,*], Sehoon Kim[3,*], Juyoung Yoon[*]

Department of Chemistry and Nanosciences, Ewha Womans University, Korea
[1]*College of Chemistry, Fuzhou University, China*
[2]*College of Pharmacy, Ewha Womans University, Korea*
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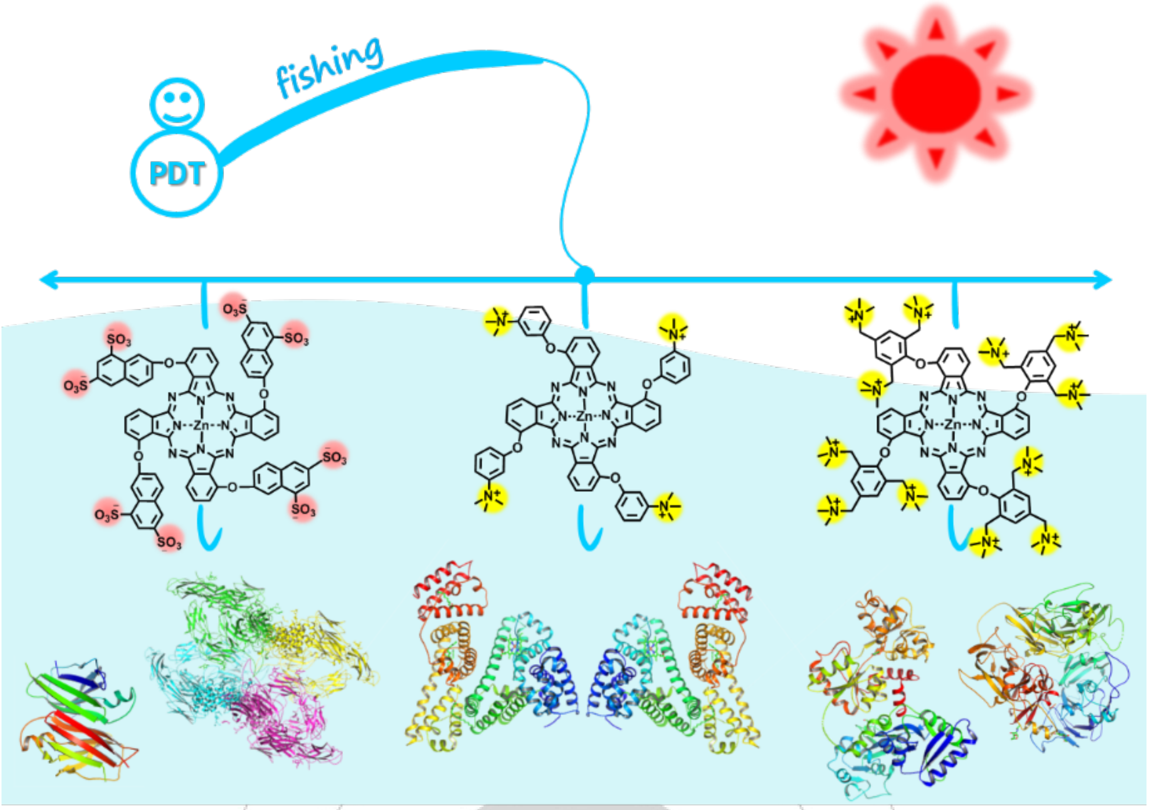
Selective delivery of therapeutic operator to target is one of the major interests in cancer treatment field. We figured out a proficient and green way to deliver phthalocyanine-based photosensitizers to tumor. Natural carrier, in-vivo albumin was applied for the delivery of photosensitizers. Unlike other phthalocyanines, which did not present selectivity towards albumin dimer and monomer, positively-charged phthalocyanine $ZnPcN_4$ showed unique specific binding with albumin dimer. The results are supported by gel assays, optical spectra and computational calculations Owing to the transport by albumin, an excellent accumulation of phthalocyanines was possible. Albumin adds a merit to this study because albumin is naturally occurring in human bodies so that unnatural additives from outside are not necessary. $ZnPcN_4$ presents an extraordinary phototherapeutic anticancer effect showing strong absorption in the far-red/near-infrared regions and generating high level of reactive oxygen species.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Poster Presentation : **ORGN.P-265**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Studies of photocatalytic artificial photosynthesis by molecular water oxidation catalyst and photosensitizer

Sungyub Song, Hyuna Kim*, Jinsung Tae*

Department of Chemistry, Yonsei University, Korea

Artificial photosynthesis is a technique which mimicks plant to make chemical energy consists of carbon. Components of artificial photosynthesis include water oxidation catalysts, carbon dioxide reduction catalysts, photosensitizers, sacrificial electron acceptors and sacrificial electron donors. We tried to concentrate on the water oxidation catalysts and photosensitizers since other efficient components are synthesized formerly. Additionally, we need to combine these catalysts to one system for the mimicking of electron transport chain of plant. We attempted to assemble efficient photosensitizer and water oxidation catalyst with module assembly method, which links catalysts to silica nano particle(SiNP) with linker molecules.

Poster Presentation : **ORGN.P-266**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Improvement of mechanical properties of silica aerogels by hybridization of organic linkers

Gahyeon Kim, Eunji Han, Jinsung Tae*

Department of Chemistry, Yonsei University, Korea

Silica aerogel is a material exhibiting various properties such as low dielectric constant, low thermal conductivity, sound insulation due to its unique pore structure. Despite these various physical properties, due to the weak mechanical properties of silica aerogel, its commercialization is not that fast. As a method of reinforcing the weak mechanical properties of silica aerorgel, previous studies have used a method of hybridizing organic materials. In this study, We synthesized several materials for the purpose of hybridization to strengthen the network of silica aerogels. Each final synthesized molecule(Linker) has a silane group that can bind to silica particles at the end, enhancing the skeleton of the aerogel. Hybrid aerogels were synthesized using an optimized synthesis method for synthesizing organic inorganic hybrid aerogels, and various analyzes were performed. As a result, it was possible to synthesize hybrid aerogels with stronger strength than silica aerogels.

Poster Presentation : **ORGN.P-267**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Conversion from Heterometallic to Homometallic Metal-Organic frameworks

Kangin Kwon, Giseong Lee, Chang Seop Hong, Hogyu Han*

Department of Chemistry, Korea University, Korea

Two new heterometallic metal-organic frameworks (MOFs), LnZnTPO 1 and 2, and two homometallic MOFs, LnTPO 3 and 4 (Ln = Eu for 1 and 3, and Tb for 2 and 4; H3TPO = tris-(4-carboxyphenyl)phosphine oxide) were synthesized, and their structures and properties were analyzed. They were prepared by solvothermal reaction of the C3-symmetric ligand H3TPO with the corresponding metal ion(s) (a mixture of Ln3+ and Zn2+ for 1 and 2, and Ln3+ alone for 3 and 4). Singe crystal X-ray diffraction analysis revealed that 1 and 3 are isostructural to 2 and 4, respectively. Thermogravimetric analysis (TGA) showed that the framework is thermally stable up to about 400 °C for 1 and 2, and about 450 °C for 3 and 4. Powder X-ray diffraction (PXRD) analysis showed their pore structure changes during drying processes. The shapes of gas sorption isotherms for 1 and 3 are almost identical to those for 2 and 4, respectively. Solvothermal immersion of 1 and 2 in Tb3+ and Eu3+ solutions resulted in the framework metal-ion exchange affording 4 and 3, respectively, as confirmed by photoluminescence (PL), PXRD, infrared (IR), and inductively coupled plasma atomic emission spectroscopy (ICP-AES) analyses.

Poster Presentation : **ORGN.P-268**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Dibenzocarbazole based bipolar host materials for phosphorescent OLEDs

Kyu Yun Chai*, Younghee Park[1], Braveenth Ramanaskanda, Sohyeon Kim[1], Leero Lee[1]

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

Two bipolar host materials, TRZDBC1 and TRZ-DBC2 were designed and synthesized with triazine acceptor and dibenzocarbazole donor. The both materials showed excellent thermal stabilities, and We have constucted green and yellow phosphorescent OLED devices. The TRZ-DBC1 based yellow device exhibited excellent current efficiency of 71.4 cd/A, which is higher than that of CBP based reference device (58.0 cd/A). The external quantum efficiency of TRZ-DBC1 and TRZ-DBC2 were 25.4% and 22.4%, respectively. Which were outstanding when compare to reference device of 19.1%. The higher triplet energy (2.71 eV) of TRZ-DBC2 used as host material for green phosphorescent OLED. The green phosphorescent OLED exhibited excellent current efficiency and external quantum efficiency of 75.9 cd/A and 24.7%, respectively. These two bipolar host materials are promising candidates for green and yellow phosphorescent OLEDs.

Poster Presentation : **ORGN.P-269**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Indolocarbazole based bipolar host material for phosphorescent and fluorescent OLED applications

Kyu Yun Chai*, Subin Oh[1], Braveenth Ramanaskanda, Hasu Jung[2], Keunhwa Kim[1]

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

The bipolar material DBTO-IN/CAR was designed and synthesized with a high yield of 64%. The synthesized material exhibited an excellent glass transition temperature of 156 °C. We fabricated two different devices, namely a green phosphorescent OLED and a non-doped bipolar fluorescent emitter. Where we used DBTO-IN/CAR as the bipolar host and fluorescent dopant. The DBTO-IN/CAR host material-based device exhibited excellent power and current efficiencies of 45.36 lm/W and 51.98 cd/A, respectively. Which were higher than that of the reference CBP-based similar device, which exhibited a lower power efficiency of 42.01 lm/W. The DBTO-IN/CAR-based green phosphorescent device revealed a good EQE of 19.03%. Moreover, the non-doped cyan emitting DBTO-IN/CAR fluorescent emitter related device also exhibited better current and external quantum efficiencies of 4.30 cd/A and 2.47%, respectively.

Poster Presentation : **ORGN.P-270**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Metal-free carbonylation of amines via TBD-CO adducts

Seul Chan Lee, Hye-Young Jang[1,*]

Energy System, Ajou University, Korea

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

Utilization of carbon monoxide (CO) with the transition metal catalysts has been widely studied and has been employed in commercial processes. For example, acetic acid synthesis, hydroformylation, Fischer-Tropsch process are known.However, most of these processes require expensive transition metal catalysts such as rhodium and iridium because carbon monoxide is not reactive without transition metal species.In this study, we focused on the carbonylation of amines in the absence of metal catalysts which has rarely been reported.To pursuit our goal, dimeric TBD-CO adducts were considered.Dimeric TBD-CO adducts was formed under pressurized CO condition, and these TBD-CO adducts were converted to formylated TBD (TBD-CHO) which played to deliver CO to organic compounds.Detailed reaction conditions and mechanistic studies including theoretical calculations (DFT) are discussed.

Poster Presentation : **ORGN.P-271**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

2,6-Disubstituted Dibenzofuran and Dibenzothiophene-Based Novel Hole Blocking Materials for High-Efficiency and Long-Lived Blue Phosphorescent OLEDs.

Seokhoon Jang, Youngu Lee*

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

Since phosphorescent organic light-emitting diodes (PhOLEDs) have four times higher quantum efficiency than fluorescent OLEDs in that they can utilize both singlet and triplet excitons, they are focused on the display market and widely used. Many studies have been conducted to enhance the performance of PhOLEDs, but satisfactory efficiency and lifetime have not been achieved for blue emitters. In order to improve the efficiency of the blue PhOLED, a hole blocking layer (HBL) can be introduced between the electron transporting layer (ETL) and emissive layer (EML). In general, the highest occupied molecular orbital (HOMO) energy level of the ETL is not much lower than that of the EML. Holes reaching the EML from an anode can be migrated into the ETL, lowering their efficiencies. Therefore, it is necessary to introduce a HBL with deep HOMO energy level. In addition, if the triplet energy (E_T) of ETL is lower than that of EML, the triplet excitons created in EML can be quenched at the interface between EML and ETL. Therefore, a HBL should have high E_T as well as deep HOMO energy level.In this work, Novel hole blocking materials (HBMs) based on 2,6-disubstituted dibenzo[b,d]furan and dibenzo[b,d]thiophene segments, 3,3',3'',3'''-(dibenzo[b,d]furan-2,6-diylbis(benzene-5,3,1-triyl))tetrapyridine (26DBFPTPy) and 3,3',3'',3'''-(dibenzo[b,d]thiophene-2,6-diylbis(benzene-5,3,1-triyl))tetrapyridine (26DBTPTPy), are rationally designed and synthesized for high-performance blue PhOLEDs for the first time. Computational simulation is used to investigate the optimal structure, orbital distribution, and physicochemical property of both molecules. Thermal, optical, and electrochemical analysis show that 26DBFPTPy and 26DBTPTPy possess high thermal stability, deep HOMO energy level (-7.08 and -6.91 eV), and E_T (2.75 and 2.70 eV). Blue PhOLEDs with 26DBFPTPy or 26DBTPTPy as a HBL exhibit low turn-on voltage (3.0 V) and operating voltage (4.5 V) at 1000 cd m^{-2}. In addition, the blue PhOLEDs with 26DBFPTPy or 26DBTPTPy show superior external quantum efficiency (24.1 and 23.6%) and power efficiency (43.9 and 42.7 lm W^{-2}). They also show a very small efficiency roll-off of about 8.5% from 100 to 1000 cd m^{-2}. Details of the correlation between the structure of organic molecules and their properties with OLED performance will be presented.

Poster Presentation : **ORGN.P-272**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Metal-free oxidation of amines and hydrocarbons

Si Ae Kim, Hye-Young Jang[1,*]

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

Aerobic oxidation in the absence of transition-metal catalysts is more sustainable and eco-friendly method compared to the metal-catalyzed chemical oxidation.However, activation of the oxygen molecule without transition metal complexes is challenging due to the stability of its triplet state oxygen.Currently reported metal-free aerobic oxidation involves the radical species to allow the triplet oxygen.1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD) can be considered as a strong base because of the resonance stabilization of the conjugate acids to react with organic compounds.The strong basicity of TBD is expected to deprotonate protons of unstable peroxide intermediated, which are formed during aerobic oxidation.Herein, we have proposed effective metal-free aerobic oxidation mediated by TBD and detailed reaction conditions and results are discussed.

Poster Presentation : **ORGN.P-273**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Heavy Atom Effect on Xanthene Dyes for Interfacial Photopolymerization by Visible Light

Young Jae Jung, JungKyu Lee*

Department of Chemistry, Kyungpook National University, Korea

We investigated the influence of heavy halogen atoms (Br and I) on xanthene dyes for interfacial polymerization based on visible-light photoredox catalysis. Since the heavy atoms directly affect intersystem crossing (ISC), which can act as a gatekeeper in the photoredox cycle and was expected to affect also intermolecular photoinduced electron transfer (PET), we attempted to quantify the influence of the halogens. Six different xanthene dyes were chosen based on the number and type of the heavy atoms on the xanthene ring. Thus, the photopolymerization degree clearly increased in this order: fluorescein < 4’,5’-dibromofluorescein ≤ 2’,4’,5’,7’-tetrabromofluorescein < 2’,4’,5’,7’-tetraiodofluorescein. Furthermore, 4’,5’-dibromorhodamine 6G showed a drastic enhancement in the photopolymerization degree, compared with rhodamine 6G. Therefore, we concluded that the presence of the halogens on the xanthene ring increases the photoredox catalytic activity due to the enhanced ISC efficiency and PET rate.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

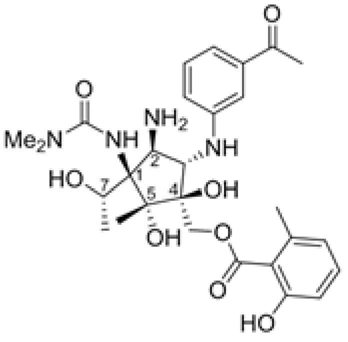
Poster Presentation : **ORGN.P-274**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

The first total synthesis and structural confirmation of pactalactam, a minor metabolite of pactamycin-producing actinomycetes

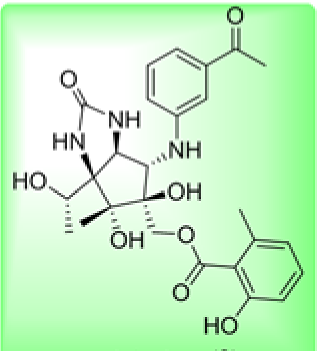
Taejung Kim, Young-Tae Park, Jungyeob Ham*

Natural Products Research, Korea Institute of Science and Technology, Korea

Pactamycin (**1**) is a representative bioactive aminocyclopentitol isolated from the culture broth of *Streptomyces pactum* var. *pactum*. Its attractive bioactivity and intriguing chemical structure based on a densely functionalized cyclopentane core drove the isolation of several related bioactive aminocyclitols. Although the development of **1** as a clinical drug has been curtailed by its broad and potent cytotoxicity, these related analogs exhibit antimicrobial, antitumor, and antiprotozoal activities, among others. However, their structure-activity relationships are not completely understood. Thus, expanding the scope of pactamycin analogs may lead to the discovery of a more acceptable safety profiles with well-characterized bioactivity. Pactalactam (**2**) was reported in a review paper published in 1980 by Rinehart *et al*. as a minor component of the metabolite of the same genus culture broth as that of **1**, but no data was available to confirm its structure. Its reported structure formula is similar to that of **1**, except for the imidazolidinone moiety; it is also analogous to that of pactamycate, an oxazolidinone derivative obtained by the acidic treatment of **1** where the 7-hydroxy group attacked the carbamoyl group. Although **2** was reported to be inactive against bacteria, these shelved analogs deserve reexamination regarding their structures and coexistence in the culture broth. Herein, we report the synthesis of the reported structure of **2** and reveal its existence in nature.



pactamycin (**1**)



pactalactam (**2**)

Poster Presentation : **ORGN.P-275**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Continuous Flow Synthesis of 1-Sulfonyl and 1-Sulfamoyl-1,2,3-Triazoles and Cu (Ⅰ)/Rh(Ⅱ) Dual Catalysis in One Flow System

Yong-Ju Kwon, Wonsuk Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

1-Sulfonyl-1,2,3-triazoles are useful compounds which can be a precursor of reactive azavinyl carbenes. Because of their weak N1-N2 bond, they can easily transform to diazoimines through ring-chain tautomerization and it leads to subsequent conversion to the metallocarbene complexes. Thus, many different batch-type methods for the preparation of 1-sulfonyl-1,2,3-triazoles have been developed. However, there is no report in flow chemistry which handled sulfonyl group substituted triazoles. Herein, we report an efficient method for the synthesis of 1-sulfonyl- and 1-sulfamoyl-1,2,3-triazoles employing continuous flow microreactor in s short residence time. In addition, we generated various substituted N-allylated (Z)-amino vinyl carboxylates with α-imino Rh(Ⅱ) carbenoids derived from triazoles by using an one integrated flow synthesis system.

Poster Presentation : **ORGN.P-276**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Design and Synthesis of Thienylthiazole Small Molecules Containing B ← N-Bridge for Organic Photovoltaic Cells

Jae-Yeon Lee, Wonsuk Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Organic materials for organic photovoltaic (OPV) have been developed to increase the power conversion efficiency (PCE). Today, small molecules for OPV have been regarded as the perfect alternative to polymer-based organic materials due to their well-defined structure, high purity, no end group contamination and excellent batch-to-batch consistency.In general, the introduction of B←N unit into π conjugated small molecules can increase E_{HOMO} and enable contraction of small molecules that exhibit large Jsc and high Voc. In addition, many groups have recently demonstrated that the B←N bridged thenylthiazole moiety can be used for photosensitive materials.Thus, based on previous studies, we designed and synthesized new A-π-D type small molecules with small band gaps and low E_{HOMO} by introducing B←N bridged thenylthiazole, triphenylamine and indanedione derivatives. Synthesized B←N-bridged thenylthiazole-containing molecules exhibit high electron affinity, which indicates band gap energy reduction and broad band absorption. In this study, a synthetic method for the preparation of B←N bridged thenylthiazole based organic photovoltaic cells and the application of their solar cells are presented.

Poster Presentation : **ORGN.P-277**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

New synthetic strategy for novel flavonoids derivatives from Houttuynia cordata.

Jeong In Yun[*], Jang Hoon Back, HyunJung Lee, Jung Youl Park[1,*]

chemistry, GH Biotech, Korea
[1]*Dept. of Applied Chemistry, Daejeon University, Korea*

Houttuynia cordata, also known as fish mint, fish leaf, rainbow plant, chameleon plant, heartleaf, fish wort, Chinese lizard tail, or bishop's weed, is one of two species in the genus Houttuynia (the other being H. emeiensis). It is a flowering plant native to Southeast Asia. Flavonoids are mainly found in natural ingredients such as fruits, vegetables, grains and flowers and are applied to various fields such as pharmaceuticals and cosmetics.Houttuynia cordata also has flavonoids structure shown that it has multiple biological activities, such as antiviral, anti-inflammatory, antibacterial, immunomodulatory, antiradiation, and antidiuretic effects. In this study, we designed and synthesis of new flavonoids derivatives from natural compounds of H.cordata.

Poster Presentation : **ORGN.P-278**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Cu-catalyzed 1,6-aza-Michael Addition of (Hetero)arylamines to 1,3-Dienes

Subin Park, Hanseul Lee, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

Metal-catalyzed conjugate additions of nucleophilic amines are of great importance for synthesis of amines with high regio- and stereoselectivity. Especially allylic amines are valuable building blocks for biologically active compounds and useful intermediates for medicinal chemistry. Nevertheless, 1,6-conjugate amine addition to dienes using metal catalysts is not well known. Therefore, we developed an efficient and selective 1,6-conjugate addition of (hetero)arylamines to sulfonyl dienes in the presence of a copper catalyst which is inexpensive, environmentally benign, and easy-to-handle. In this methodology, reactivity and regioselectivity were successfully controlled using a sterically demanding NHC ligand to afford 1,6-addition products. The amination was promoted by the presence of 7.5 mol % NHC-CuCl and 7 mol % KOt-Bu and selectively proceeded to complete conversion in toluene, affording sulfonyl-substituted allylic amines. This catalytic process provided versatile and new allylic amines in high yields with excellent regioselectivity. In addition, the sulfonyl-substituted amine product obtained from our methodology was applied to the cyclization to prepare diphenyl, terphenyl and cyclopropane compounds.

Poster Presentation : **ORGN.P-279**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Stereoselective Synthesis of 2-Alkyl-1,3,3-Trinitroazetidine Derivatives

Bora Kim, Chang-Woo Cho*

Department of Chemistry, Kyungpook National University, Korea

1,3,3-trinitroazetidine has attracted significant attention as an important energetic material in the defense industry because of its low melting point and good thermal stability in the melt phase. For this reason, active research has been pursued on methods for the synthesis of 1,3,3-trinitroazetidine. Despite the potential application of 2-substituted-1,3,3-trinitroazetidines in propellants and plasticizers, there is no known report of their synthesis, presumably due to the challenges posed by the highly strained ring system. Recently, as an example of the application of energetic materials in medicine, 1-bromoacetyl-3,3-dinitroazetidine has been developed as an anticancer agent and is undergoing Phase III clinical trials. Since 2-substituted-1,3,3-trinitroazetidines are also applicable as potential candidates of medicinal substances as well as propellants and plasticizers, the development of an asymmetric synthetic route to produce enantiopure 2-substituted-1,3,3-trinitroazetidines is highly desirable. Here, we report the efficient synthesis of diverse enantiopure 2-substituted-1,3,3-trinitroazetidines. We also investigate the effect of the C2 alkyl substituent on the sensitivity of 2-substituted-1,3,3-trinitroazetidines as high-energy materials.

Poster Presentation : **ORGN.P-280**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Stereoselective Synthesis of Chiral Pyrimidine Acyclonucleosides by Organocatalytic Aza-Michael Reaction

Heun-Jong Ha, Chang-Woo Cho*

Department of Chemistry, Kyungpook National University, Korea

Pyrimidine acyclonucleosides have received considerable attention because of their appealing biological activities. In particular, owing to the importance of the absolute configuration of the stereogenic carbon center in the side chain of chiral pyrimidine acyclonucleosides, few asymmetric catalysis strategies for the synthesis of chiral pyrimidine acyclonucleosides have been reported recently. However, while the use of pyrimidines as *N*-centered nucleophiles in the transition-metal-catalyzed asymmetric reactions has been researched, the corresponding use of pyrimidines in organocatalytic asymmetric reactions remains unexplored. Here, we report an efficient and highly enantioselective organocatalytic aza-Michael reaction of pyrimidines as *N*-centered nucleophiles to α,β-unsaturated aldehydes that affords the desired chiral pyrimidine acyclonucleosides.

Poster Presentation : **ORGN.P-281**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Development and Bioactivity Evaluation of New Anticonvulsants with Valproic Acid Derivatives

Songmi Bae, Dai Il Jung*, Ju Hyun Song

Department of Chemistry, Dong-A University, Korea

Epilepsy is the result of temporary brain dysfunction in parts of the brain or parts of the brain. The exact mechanism of epilepsy is unknown, but a little is known about the cell and network mechanism. With regard to the development of new anticonvulsants, we investigated the structural similarity of various anticonvulsants known to work by different mechanisms. So we designed an active structure like ester and acid anhydride as a new anticonvulsant in a wider spectrum of one molecule. Ester and acid anhydride, substances we synthesized, represent physiological activity before they are separated by cations and anions with physiological activity, separated by the original active substance and delivered to the blood when administered in the body. This reaction process has been applied to develop materials with good anticonvulsants as well as those with low side effects. Using this method, which we named "Niche chemistry", we created new drugs by synthesizing acids (valproic acid, lauric acid, palmitic acid, decanoic acid, caffeic acid, salicylic acid, aspirin… etc) with anticonvulsant effects and some alcohols(resveratrol, acetaminophen…etc) with antiepileptic effects. We will report the evaluation of in vivo and in vitro anticonvulsants of valproic acid derivatives among the synthesized product.

Poster Presentation : **ORGN.P-282**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Copper-Catalyzed Hydroamination of Anilines with Allylic Sulfones

Kundo Kim, Subin Park, Yunmi Lee[*]

Department of Chemistry, Kwangwoon University, Korea

The synthesis of β–amino sulfone compounds is significant because of its applications to natural products, drugs, and functional materials. In addition, β-amino sulfones are important intermediates in the preparation of cyclic or acyclic nonproteinogenic α-amino acids, amines and alkaloids, taking advantage of the fact that sulfones can be readily functionalized. One of the efficient methods for synthesis of β–amino sulfones is Cu-catalyzed hydroamination with sulfonyl-substituted alkenes. Therefore, in this presentation, we described a new and regioselective hydroamination of anilines with allylic sulfones promoted by an NHC-Cu catalyst. Our methodology is attractive due to the use of cheap and easy-to-handle copper catalyst and the use of readily available allylic sulfone starting materials. The amination was carried out in the presence of NHC-CuCl and KOt-Bu under mild reaction conditions, providing a broad range of β-amino sulfones in high yields with excellent regioselectivity.

Poster Presentation : **ORGN.P-283**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and characterization of amino-oxy modified Sphingosine-1-phosphate (S1P) derivative that can replace thiolated-S1P in competitive ELISA

Ji hye Park, Yongtae Kim, In seok Hong*

Department of Chemistry, Kongju National University, Korea

Sphingosine-1-phosphate (S1P) is a signaling molecule that plays various roles in vivo. Recently, S1P has emerged as a biomarker in the early diagnosis of osteoporosis and cancer. A competitive ELISA assay kit for detecting S1P in blood or in various samples is now commercially available. Competitive ELISA requires anti-S1P antibody and S1P-coated microtiter plates. The antigenic derivative used here is the thiolated-S1P in which a sulfur hydryl group is introduced at the terminal end of the S1P hydrophobic chain. However, the sulfur hydryl group is easily oxidized, and its solubility in water is considerably low, making it difficult to handle. In this study, amino-oxy modified S1P derivatives that can replace thiolated-S1P were synthesized. Amino-oxy groups are easy to attach to proteins and other polymers without any linker, and are easy to handle because they are not easily oxidized, and soluble in water. The synthesized S1P derivative was directly immobilized on a microtiter plate and ELISA assay was performed to obtain comparable results with the conventional thiolated-S1P reference. It is expected that anti-S1P antibody can be easily induced by attaching this amino-oxy modified S1P to reduced carrier proteins.

Poster Presentation : **ORGN.P-284**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Tandem C−H Allylation and [3+2] Dipolar Cycloaddition under Ruthenium(II) catalysis

Heeyoung Lee, In Su Kim[1,*]

School of Pharmacy, Sungkyunkwan University, Korea
[1]*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The ruthenium(II)-catalyzed C–H functionalization of (hetero)aryl azomethine imines with allylic acetals is described. The initial formation of allylidene(methyl)oxoniums from allylic acetals could trigger C(sp^2)–H allylation, and subsequent endo-type [3+2] dipolar cycloaddition of polar azomethine fragments to deliver valuable indenopyrazolopyrazolones. This is the first example of using allylic acetals as highly electrophilic acrolein oxonium precursors in C−H allylation, which results in the formation of a synthetically useful enol ether moiety for further transformations. Due to their equilibrium under metal catalysis, allylic acetals might serve as highly activated acrolein oxonium precursors for cross-coupling reactions.The utility of this method is showcased by the late-stage functionalization of bioactive molecules such as estrogen and celecoxib. Combined experimental and computational investigations elucidate a plausible mechanism of this new tandem reaction. Notably, the reductive transformation of synthesized compounds into biologically relevant diazocine frameworks highlights the importance of the developed methodology.

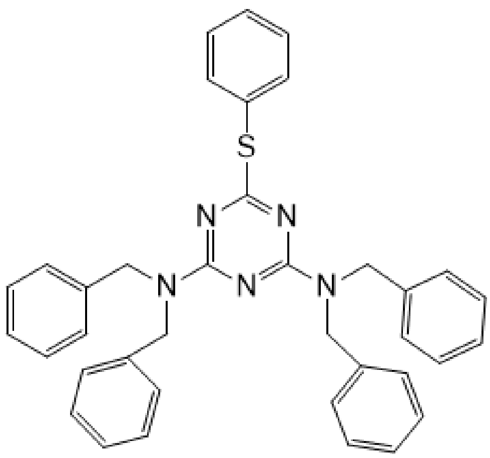
Poster Presentation : **ORGN.P-285**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Sulfur and Sulfonyl substitution effect on the C-N Bond Rotation of Dibenzylamino-1,3,5-triazines

Joonho Kim, Yeong-Joon Kim*, Jaehee Song[1]

Department of Chemistry, Chungnam National University, Korea
[1]*Department of Chemistry, Suncheon National University, Korea*

Dibenzylamino-1,3,5-triazine derivatives (**1, 2**) were synthesized from 2,4,6-trichloro-1,3,5-triazine and dibenzylamine to as starting materials, and then introducing S-Phenyl or S-butyl substituents. Other derivatives (**3, 4**) were synthesized from the reaction of **1** (or **2**) and peroxide hydrogen. The C-N bond rotational energy of the compounds in DMSO-d_6 and Toluene-d_8 was obtained by using variable-temperature ^{1}H-NMR. ^{1}H-NMR spectra showed two benzyl signals at room temperature and two peaks coalesced at higher temperature. The activation energies ($\Delta G^‡$, $\Delta S^‡$, $\Delta H^‡$) were calculated through the coalescence temperature method and line shape analysis. Electronic effects of the sulfur and sulfonyl will be discussed using Hammett plot.



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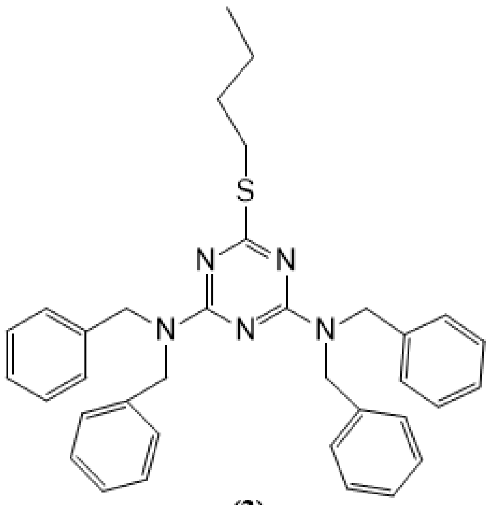

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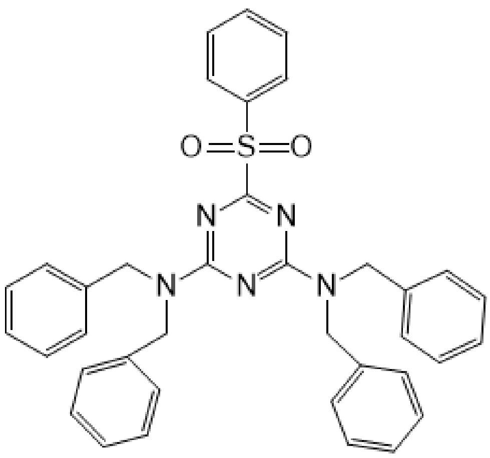

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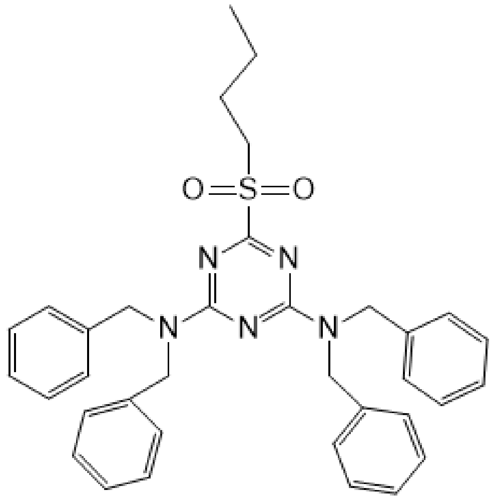

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Poster Presentation : **ORGN.P-286**

Organic Chemistry

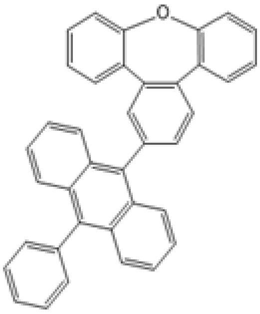
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of compounds containing oxepine and phenylanthrancene for the use of OLED materials

<u>Joonho Kim</u>, Yeong-Joon Kim*

Department of Chemistry, Chungnam National University, Korea

OLED materials mostly consist of aromatic rings. In this work, we would like to introduce the oxepine compounds can also be used as OLED materials. Oxepine was obtained by an intramolecular nucleophilic substitution reaction of 2,2'-Fluoro-hydroxy-o-tertphenyl. Compound (**1**) and (**2**) were synthesized by Suzuki-Miyaura reaction of oxepine-boronic acid and phenylbromoanthrancene. These compounds are expected to be used as OLED HOST materials.



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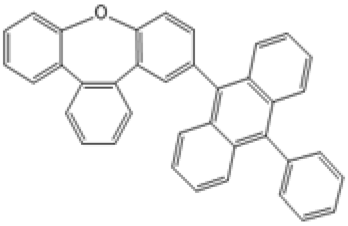

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Poster Presentation : **ORGN.P-287**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Design and Synthesis of Transglutaminase 2 Inhibitors to Improve Isozyme Selectivity

Sol Han, Suhyeon Min, Kihang Choi[1,*]

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

Transglutaminase 2 is one of the nine members of the transglutaminase family that catalyze crosslinking reactions between protein glutamine and lysine residues in two steps. First, the thiol group of Cys277 at TG2 active site reacts with a glutamine substrate to form a thioester intermediate. Then, this enzyme-substrate complex reacts with a lysine substrate to generate the crosslinking product. Because TG2 is involved in several diseases such as celiac disease, neurodegenerative diseases and cancers, many TG2 inhibitors have been studied as a potential treatment option for these diseases. Most of these are glutamine-substrate mimics targeting Cys277 at the active site. Among these Transglutaminase family, TG2 has a lysine residue near to the Cys277. To improve the isozyme selectivity, we synthesized compounds that have two electrophilic moieties, one to react with Cys277 and the other to target the Lys residue at the same time. Appropriate biological TG2 activity assay was performed to test the inhibitory efficiencies of the synthesized compounds. Our work suggests a new strategy to develop TG2 inhibitors with improved selectivity.

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Poster Presentation : **ORGN.P-288**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Transfer Hydrogenation of inorganic carbonates with Glycerol

Kihyuk Sung, Yeon Joo Cheong, Hye-Young Jang[1,*]

Department of Energy System, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

As the biodiesel industry grows, the production of glycerol, the main by-product, is also increasing. Glycerol, which is non-toxic, inexpensive and biodegradable, can be used as a solvent and a hydrogen source in the transfer hydrogenation instead of explosive H_2 gas. Many researches have been achieved on the catalytic activity of iridium complexes in transfer hydrogenation. We aimed to develop a catalytic conversion for reducing CO_2 while glycerol was used as a liquid hydrogen. By this research, CO_2 emission can be reduced and chemical waste can be converted to valuable products.

Poster Presentation : **ORGN.P-289**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A fluorescent probe for the sequential detection of nitroreductase and nitric oxide under hypoxic condition

Jung Won Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Hypoxia means a condition in which the human body is deprived of enough oxygen supply at the tissue level. It is one of the special features of tumor physiology. Increasing biological activity of nitroreductase (NTR) is well-known phenomenon in hypoxic tumors. So, level of NTR is a crucial factor for monitoring hypoxic degree in tumors. In addition, hypoxia causes increasement of nitric oxide (NO) generation. NO plays in the improvements of blood flow and oxygen supply in hypoxic conditions. Therefore, both NTR and NO are important factors for monitoring hypoxia more precisely. But little research has been done to detect them by a single system. The development of a probe which can detect two representative tumor-specific factors is important and meaningful for biological applications. In order to detection of both NTR and NO by a single system, we designed a fluorescent probe for the sequential detection of NTR and NO. For targeting NTR and NO, nitroaromatic and diamino aromatic moieties were used as a sequential reactive site. In the presence of NTR and NO, this probe undergoes the sequential nitro reduction and triazole ring formation. This shows distinct fluorescence changes, providing a selective and sensitive imaging of hypoxic conditions in living cancer cells. We investigated the detailed spectroscopic properties of the probe to NTR and NO. Recently, the validation of probe's detection ability is ongoing in the hypoxic and normoxic cancer cells.

Poster Presentation : **ORGN.P-290**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Off-On fluorescent probe for imaging cancer-specific hNQO1 in living cells

Sun Young Park, Eugeine Jung[1], Jongseung Kim[2], Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea
[1]*Department of Life Sciences, Korea University, Korea*
[2]*Department of Chemistry, Korea University, Korea*

Human NAD(P)H:quinone oxidoreductase 1 (hNQO1) is a cancer-specific biomarker, which is overexpressed in cancer cells and also associated with a drug resistance factor of cancer. Herein, we presented hNQO1-responsive fluorescent Off-On naphthalimides **1** and **2** that could be employed for imaging hNQO1 activity in living cancer cells. Upon the presence of hNQO1 activity, the naphthalimides gave rise to a strong fluorescence Off-On change at 540 nm. In hNQO1-positive A549 cells, the naphthalimides showed a strong fluorescence image through a hNQO1-mediated enzymatic reaction, in contrast to hNQO1-negative H596 cells and hNQO1 inhibitor-pretreated A549 cells. We could propose that naphthalimides **1** and **2** can be used for a real-time monitoring of hNQO1 activity in living cancer cells.

Poster Presentation : **ORGN.P-291**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A development of red-emitting fluorescent probes for NAD(P)H and its use for the real-time imaging in cancer cells

Jin Hui Joo, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Reduced nicotinamide adenine dinucleotide (NADH) and its phosphate ester (NADPH) are the factors involving in many redox reactions in living cells. In particular, the NAD(P)H plays a crucial role as universal electron carrier in cellular processes. NAD(P)H and NAD(P)$^+$ undergo reversible oxidation–reduction in many biological reactions. When NAD(P)H is defective, it causes degenerative diseases such as Parkinsonism and Alzheimer's disease. In this regard, we developed NAD(P)H targetable probes **1** and **DCQ**. Previously, our group developed a red-emitting fluorescent probe (**1**) based on dicyanoisophorone for monitoring of mitochondrial NAD(P)H in cells. This probe was successfully used to selectively detect endogenous NAD(P)H in cells, but it required relatively long reaction time. So, we developed a new fluorescent probe (**DCQ**) based on dicyanocoumarin with far red-emitting and fast reaction time for NAD(P)H detection. We think that it would be suitable for real-time monitoring of NAD(P)H in living cells. Furthermore, we monitored the fluctuations of cellular NAD(P)H by using the glucose-stimulated endogenous NAD(P)H increase model and pyruvate-induced endogenous NAD(P)H depletion model. We envisioned that **DCQ** will be useful to elucidate biological pathways, pathological diagnosis and other applications by selective imaging of NAD(P)H.

Poster Presentation : **ORGN.P-292**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A naphthalimide based turn-on fluorescent probe for detection of nitric oxide in living cells

Su Jung Kim, Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Nitric oxide (NO) is generated from L-arginine through nitric oxide synthase (NOS) in living cells. NO plays a crucial role in diverse biological processes such as vasodilation, carcinogenesis, neurodegenerative disorders, and neurotransmission. In this regard, we developed naphthalimide-linked thiosemicarbazide as a turn-on fluorescent probe for NO detection. This probe is almost non-fluorescent presumably by the fluorescence quenching process through a free rotation of thiosemicarbazide moiety. However, the probe gave a turn-on fluorescence signal upon treatment of NO. We found that the thiosemicarbazide moiety of probe can react with NO to produce a highly fluorescent naphthalimide. The detection limit turned out to be as 0.22 μM. In addition, the selectivity of probe toward NO over reactive oxygen species, reactive nitrogen species, and metal ions was demonstrated. Moreover, this probe was applied for the detection of exogenous and endogenous NO in living cells.

Poster Presentation : **ORGN.P-293**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A coumarin-appended naphthalimide ratiometric fluorescent probe for detection of nitroreductase and its application to live cells.

Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Nitroreductase (NTR) are flavoenzymes that catalyze the NAD(P)H-dependent reduction of the nitro groups on nitroaromatic compounds. It assumed that they play a key role in the detoxification of carcinogens because most nitroaromatic compounds are toxic and carcinogenic for living systems. In addition, it is reported that the NTR activity is increased in human tumor cells and it is widely employed in prodrug activation for chemotherapeutic cancer therapy. In this work, coumarin-appended naphthalimide ratiometric fluorescence probe **1** was developed for detection of nitroreductase. Probe **1** showed the fluorescence emission at 475 nm as a coumarin moiety. However, in the presence of NTR, new emission band at 550 nm was emerged and coumarin emission at 475 nm was showed negligible change. Also, we could plot fluorescence intensity ratio ($I_{550\text{ nm}}/I_{475\text{ nm}}$) and the limit of detection for was calculated to be 3.78×10^{-4} μg/mL. Moreover, the kinetic parameters for the enzymatic reaction of probe **1** towards NTR, determined by using Michaelis-Menten analysis were found to be Michaelis constant (K_m) = 23.44 ± 8.64 μM, maximum velocity (V_{max}) = 3.42 ± 0.83 μmol min^{-1} mgNTR^{-1}, catalytic constant (k_{cat}) = 1.36 ± 0.33 s^{-1}, and specificity constant (k_{cat}/K_m) = $5.82 \text{ x } 10^4 \pm 0.03$ M^{-1} s^{-1}. We also confirmed the product after the reaction of NTR using mass analysis and high-performance liquid chromatography (HPLC). Additionally, encouraged by the excellent photophysical properties, we are planning to conduct a cell experiment using probe **1**.

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Poster Presentation : **ORGN.P-294**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A development of ratiometric fluorescent probe for imaging of hydrazine

Minjoo Jung, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

We synthesized an AIEgen-based fluorescent probe capable of selectively sensing hydrazine. Due to its gas phase, it is easy to be exposure to hydrazine, through the skin, breathing and oral cavity. Besides hydrazine damage to the central nervous system and cause infections of the respiratory. So, monitoring hydrazine is important because of these harmful characteristics. TPE (tetraphenylethane) is one of the well known aggregation-induced emission luminogens (AIEgens), AIEgens have advantages such as high quantum yield, photostability, and large stokes shift. Because of these advantages, our probe was designed based on TPE. Dicyanovinyl groups as a strong electron acceptor and N, N-dimethylamino groups as a electron-donating groups, were introduced into TPE probes with donor-acceptor (D–π–A) systems. It is expected that the dicyanovinyl group will act as a moiety to target hydrazine to form dimers, and that it will be able to selectively detect hydrazine with blue shift.

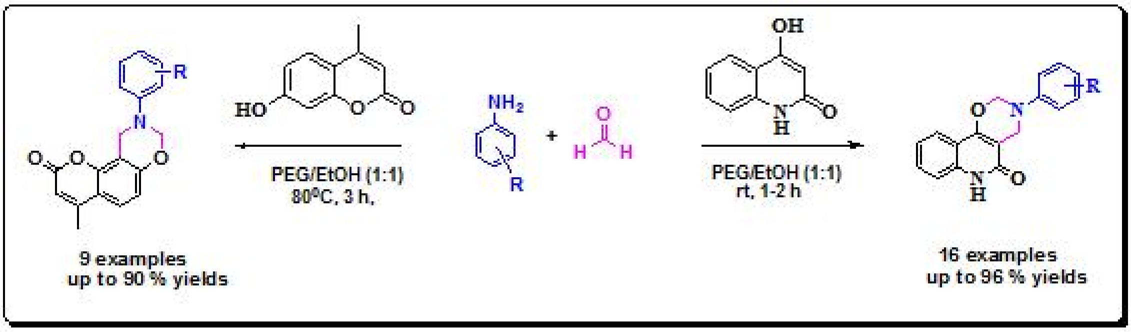
Poster Presentation : **ORGN.P-295**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

PEG-assisted One-pot three-component synthesis of [1, 3] Oxazino [5, 6-c] quinolin-5-one and 4-methyl-9-phenylchromeno [8, 7-e] [1, 3] oxazin-2(8H)-one under catalyst free condition

Maruti Yadav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

PEG-assisted solvent and eco-friendly straightforward synthesis of [1, 3] Oxazino [5, 6-c] quinolin-5-one and 4-methyl-9-phenylchromeno [8, 7-e] [1, 3] oxazin-2(8H)-one via three component cascade reaction of various aromatic amine with formaldehyde using very mild and catalyst free reaction conditions. The merit of this protocol is highlighted by its easily available and economical starting materials, operational simplicity, and clean reaction profile, simple workup procedure, and tolerance of a wide variety of functional groups.



Poster Presentation : **ORGN.P-296**

Organic Chemistry

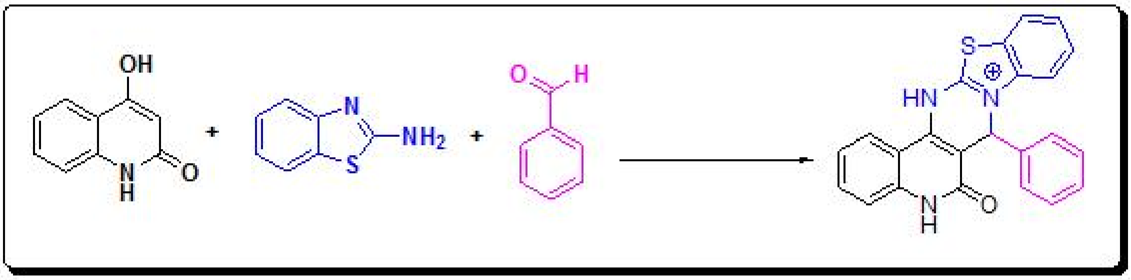
Exhibition Hall 1, FRI 11:00~12:30

Highly efficient and cascade synthesis of densely functionalized quinoline alkaloids under catalyzed reaction conditions

Maruti Yadav, Yeon Tae Jeong*

Department of Display Engineering, Pukyong National University, Korea

A simple, eco-friendly, and cost-effective method has been disclosed for the synthesis of 6-oxo-7-phenyl-5,6,7,14-tetrahydrobenzo[4',5']thiazolo[3',2':1,2]pyrimido[5,4-c]quinolin-8-ium under catalyzed reaction condition. This reaction is a versatile one-pot multicomponent condensation of 4-hydroxyquinoline, 2-aminobenzothiozoles, and various aldehydes. 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.



Poster Presentation : **ORGN.P-297**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Two-photon Probe for TNF-α. Detection of Human Colon Inflammation by Two Photon Microscopy

Byumseok Koh, Eunyoung Yoon, Jung-Nyoung Heo[1,*], Bong rae Cho[2,*]

Korea Research Institute of Chemical Technology, Korea
[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*
[2]*Department of Chemistry, Daejin University, Korea*

Inflammatory bowel diseases (IBD), consisted of two major illness such as ulcerative colitis (UC) and Crohn’s disease (CD), are disorders that involve the chronic inflammation of the intestinal mucosa. However, there is difficult to direct diagnosis method for detecting cancer cells in human colon tissues. TNF-α(tumor necrosis factor-α) play a role in diagnostic indicator of cancer, and targeting TNF-α might be a promising prognostic tool by assessment of the clinical stages of IBD. Two-photon imaging is a powerful technique for the diagnosis of cancer cells because observable deep into tissue.In this study, we focuse on a two-photon probe for TNF-α that can be applied in human colon tissues. We have developed a two-photon probe for TNF-α by conjugating Pyr1 moiety with infliximab (Pyr-infliximab). Our Pyr-infliximab exhibited characteristics high selectivity, no cytotoxicity TNF-α in a live cell and human colon tissue by Two photon microscopy. Further our design strategy can provide a guideline for generating two-photon biomarker that target disease-related proteins with high selectivity and specificity.

Poster Presentation : **ORGN.P-298**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

A Solvent- and Metal-Free Method for Preparation of *N*-Aryl-Substituted Azacycles from Arylamines and Cyclic Ethers Using Phosphoryl Chloride

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

N-Substituted azacycles have played a very important role in medicinal chemistry as well as organic chemistry field. *N*-substituted azacycle moieties were found in a lot of organic compounds such as vitamins, antigens, and alkaloids. In recognition of widespread importance of *N*-substituted azacycle motifs, there have been several studies to develop a new method to prepare *N*-substituted azacycle compounds. It was reported that some studies used transition metal salts as effective catalysts for this process. Herein, we present a direct method for the preparation of *N*-aryl substituted azacycles from arylamines and cyclic ethers without solvent and transition metal salts. Phosphoryl chloride and DBU were used as effective reagents for synthesis of *N*-substituted azacyles. Five-membered cyclic ethers such as tetrahydrofuran, and 2-methyl-tetrahydrofuran, and six- membered cyclic ethers such as tetrahydro-2H-pyran and isochroman were employed to react with arylamines without solvent, and a series of *N*-aryl substituted azacycles was synthesized in excellent yields. The efficient and economic method provided a potential approach for the synthesis of *N*-aryl substituted azacycles using cyclic ethers.

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Poster Presentation : **ORGN.P-299**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

The Directly Conversion of *N*-Troc-Cabamates to Ureas Using Catalytic CaI_2

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Chonbuk National University, Korea

Urea unit is important in pharmaceutial research. A green and practical method has been developed for the synthesis of ureas from *N*-Troc-protected amines. Multiple reagents including alkali metals and alkaline earth metals were investigated to discover an efficient catalyst to yield ureas, and CaI_2 was demonstrated as an effective catalyst for the direct reaction of *N*-Troc-carbamates to produce target urea units. Troc-protected aromatic and aliphatic amines were used as substrates to yield the target products. Under the optimized reaction conditions, CaI_2-catalyzed synthetic procedure provided the desired ureas without byproducts in excellent yields. During urea formations, CaI_2 was proven as a high level of an efficient and environmental-friendly catalyst. The CaI_2-catalyzed synthetic method can provide a new way of synthesis of many ureas.

Poster Presentation : **ORGN.P-300**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Cooperative Stereocontrol by Proximal and Distal Chlorine Substituents in the Chiral Lewis Base-Catalyzed Kinetic Resolution of *cis*-Vinyl Epoxide

Jungi Jung, Won-jin Chung*

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

Vinyl epoxides are versatile precursors to highly functionalized organic compounds.[1] Because of the high utility of vinyl epoxide, various synthetic methods and strategies have been studied and applied to total synthesis of natural products. Nevertheless, enantioselective synthesis of vinyl epoxide is challenging and typically depends on enantioselective oxidations of a limited types of unsaturated substrate. Kinetic resolution can be employed as an alternative strategy when no general, enantioselective synthetic method is available. Kinetic resolution has been successfully utilized for the synthesis of highly enantioenriched vinyl epoxide intermediates in total syntheses of chlorosulfolipids.[2] Interestingly, the selectivity factor of the kinetic resolution was dependent on the configurations of the chlorine-bearing stereocenters. [3] To explain this selectivity difference, several control experiments and computational mechanistic investigation were carried out. [4]

References

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Poster Presentation : **ORGN.P-301**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Simple Isothiouronium salt type organocatalyst for transfer hydrogenation of 2-substituted quinoline derivatives

Sungmin Kang, Taek Hyeon Kim*

School of Chemical Engineering, Chonnam National University, Korea

Simple Isothiouronium salt type organic catalyst was employed to catalyze the transfer hydrogenation of 2-substituted quinoline using Hantzsch ester as a hydrogen source. Organic catalysts of the simple isothiouronium salt type with strong hydrogen bonding ability was successfully accomplished with excellent yields and fast reaction rates.

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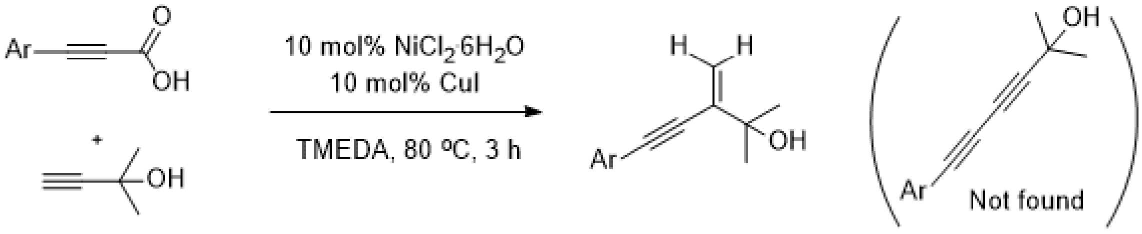
Poster Presentation : **ORGN.P-302**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of gem-1,3-Enynes: Ni/Cu-Catalyzed Decarboxylative Dimerization of Alkynoic Acids and Terminal Alkyne

Hyojin Jeon, Sunwoo Lee[*]

Department of Chemistry, Chonnam National University, Korea

Conjugated 1,3-enynes are important structural units in synthetic chemistry, material science and bioactive product synthesis. 1A number of synthetic methods have been reported for the preparation of 1,3-enynes, 2-3including Wittig reaction with propargyl aldehydes, dehydration of propargyl alcohols.We developed the synthesis of gem-1,3-enyne via Ni/Cu catalyzed decarboxylative dimerization of alkynoic acid and terminal alkyne. We found that the decarboxylation of alkynoic acid provided predominantly gem-1,3-enyne instead of 1,3-diyne which was known to be formed from the coupling of terminal alkynes. A variety of gem-1,3-diynes were obtained with good yields from the reaction of substituted aryl propiolic acids and terminal alkynes such as 2-methylbut-3-yn-2-ol, pent-4-yn-1-ol, 1-phenylpro-2-yn-1-ol, 1-entynylcychohexanol and ethynylcyclohexane. This catalytic system exhibited excellent regioselectivity and high functional group tolerance. It was found that nickel catalyst suppressed the pathway of the coupling of alkynes which was dominated by copper catalyst. This result was completely different from the previous reports 4-5which 1,3-diyne was formed from the hetero cross coupling of two different alkynes in the presence of Ni/Cu or Cu catalyst.



Poster Presentation : **ORGN.P-303**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Multi-modal stimuli-responsive poly(2-oxazoline)-based supramolecular hydrogel

Jieun Baek[*], **Woo-Dong Jang**

Department of Chemistry, Yonsei University, Korea

The researches on multi-functional hydrogel are increasingly attractive for various application fields. Boronic acid and diols can form reversible boronic ester bond, which can be used as the motif for self-healing materials. It is known that this complexation between boronic acid and diols occurs in basic condition, whereas it can be decomposed in acid condition. Therefore, it can be used as pH responsive material. Furthermore, phenylboronic acid shows fructose sensitivity. We made multi-responsive gel using poly(vinylalcohol)(PVA) and poly(2-oxazoline) containing phenylboronic acid at the end. PVA serves as diol for boronic ester formation and the oxazoline serves as the thermo-responsive component because oxazoline have lower critical solution temperature(LCST). This hydrogel showed pH, fructose, and temperature responsive and self-healing properties.

Poster Presentation : **ORGN.P-304**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Study on Improvement of TKX-50 Synthetic Method

Su-jin Oh, Yeong-Gweon Lim*

Agency for Defense Development, Korea

Dihydroxylammonium-5,5'-bistetrazole-1,1'-diolate (TKX-50) is a promising candidate to replace traditional explosive, 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) due to its high performance, insensitivity and environmentally friendly property. However, handling highly toxic reagents and unstable intermediates are the considerable challenges to resolve for large-scale or industrial manufacture. In the present study, we developed a safe and efficient synthetic route for TKX-50 by improving the existing synthetic method. Specifically, the use of toxic Cl_2 gas has been excluded by replacement of glyoxime (GLY) intermediate with diaminoglyoxime. In the diazidoglyoxime (DAG) cyclization, the key step in this process, we use the 37% aqueous solution instead of unfavorable HCl gas and improved yield and safety. this synthetic mehtod did not need to dry DAG completely and could avoid the use of non-volatile solvents such as DMF and NMP.

Poster Presentation : **ORGN.P-305**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Simple Synthesis Of Heterocyclic Compounds Via Oxidative Deacetylation Reaction

Tingshu Wang, Sangho Koo[1,*]

Department of Energy Science and Technology, Myungji University, Korea
[1]*Department of Chemistry, Myungji University, Korea*

Efficient synthetic method of medicinally and opto-electronically important bichalcophenes was proposed, which highlighted Mn(III)/Co(II)-catalyzed oxidative deacetylation of 1,5-dicarbonyl compounds, that was easily prepared by conjugate addition of ethyl acetoacetate to □,□-unsaturated carbonyl compounds containing a chalcophene unit. Paal-Knorr reactions of the resulting 1,4-dicarbonyl compounds produced 4-phenyl-2,2′-bichalcophenes and their aza-analogues.Using these method, the starting material for one pot syntheses of multi-substituted furan, thiophene, and pyrrole were easily gained. Further work on extending this catalytic oxidative reaction to the synthesis of some natural products is ongoing.

Poster Presentation : **ORGN.P-306**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Bromoacetate Olefination Protocol for Norbixin and Julia−Kocienski Olefination for Its Ester Syntheses

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Department of Chemistry, Myongji University, Korea
[1]*Department of Chemistry, Myungji University, Korea*

Norbixin 1 was efficiently produced by coupling of ethyl bromoacetate with C20 dialdehyde 6 and following double elimination of the protected hydroxyl groups and bromine atoms of the coupling bromohydrin product. Synthesis of norbixin ethyl ester 2 by Julia−Kocienski olefination of novel C7 benzothiazolyl-sulfone 11 and C10 2,7-dimethyl-2,4,6-octatrienedial 12 also was demonstrated. These two concise pathways led to 35% and 36% overall yield of norbixin 1 and norbixin ethyl ester 2, respectively.

Poster Presentation : **ORGN.P-307**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Fast Assembly and High-Throughput Screening of Structure and Antioxidant Relationship of Carotenoids

Gaosheng Shi, Sangho Koo[1,*]

Department of Energy Science and Technology, Myungji University, Korea
[1]*Department of Chemistry, Myungji University, Korea*

C20 heptaenyl diphosphonate 4 was prepared for one-pot synthesis of carotenoids 1. Olefination with various aromatic aldehydes allowed fast assembly of the corresponding carotenoids. The SAR of carotenoids was investigated by high-throughput screening of ABTS and DPPH assays and their hierarchical clustering analysis. Antioxidant activity of carotenoids increased with the number of electron-donating substituents. Carotene 1a with multiple electron-donating substituents was most proficient, which showed better radical scavenging activities than β-carotene and lycopene

Poster Presentation : **ORGN.P-308**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Research of on the synthetic methodsynthesis of Unnatural carotenoids

Bo-ram Lim, Sangho Koo[*]

Department of Chemistry, Myungji University, Korea

Unnatural carotenoids containing various phenyl substituents has show excellent characteristics in terms of stability and as well as electronic conductance. We have developed a series of efficient synthetic methods of natural carotenoids, thatwhich can be further extended to the synthesis of the unnatural stabilized carotenoids as a molecular wire. Our synthetic strategy is based on the sulfone-mediated coupling with dialdehyde and double elimination reaction. So, It is necessary to design efficient building blocks ; Under the sequence of Indium mediated addition of haloallylic sulfone and Oxonia-cope rearrangement reaction, allyic sulfone unit containing aromatic substituents can be readily prepared from Acetophenone acetophenone derivatives. And dialdehyde unit could be easily onbtained. The unnatural carotenoids can be synthesized by the coupling/double elimination reaction between allylic sulfone unit and dialdehyde unit , Protecting reaction and double elimination reaction. Therefore, we were able to measure electrical conductivity using for the unnatural carotenoid wires.

Poster Presentation : **ORGN.P-309**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of unnatural carotenoids with good electrical properties

Huijung Yang, **Sangho Koo**[1,*]

Department of Energy science and Technologe, Myungji University, Korea

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

Carotenoids have a variety of beneficial effects and are particularly good at antioxidant activity. unnatural carotenoids substituted with phenyl groups have good electrical properties in addition to their advantages. Using these advantages, the electrical conductivity can be measured by replacing the terminal group with a methylthio group and attaching to the gold plat. This unnatural carotenoids can be efficiently synthesized by the julia-kocienski olefination of triene dialdehyde with BT(benzothiazole)-Sulfone. It can assemble the methylthio group through a wittig reaction with 4-thiomethylbenzyl phosphonium bromide.

Poster Presentation : **ORGN.P-310**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of various Pyrrole compound from Amino acid and Reducing sugar

Soohyeon Cho, Sangho Koo[1,*]

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

5-(Hydroxymethyl)-2-furfural(5-HMF) is well known as an important platform chemical in biomass industry. We tried to obtain 5-HMF by conversion of monomeric sugars. We have added an amino ester to assist the ring opening and rearrangement of D-glucose with Amadori and Mailard reations. As a result, Sedative and anti-inflamnatory pyrrolo-lactone compounds were obtained which can be extracted from natural plants as folk medicine.

Poster Presentation : **ORGN.P-311**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and application of Ir(III)-(bis-NHC) Complexes : the Effect of Carboxylate Ligand on Catalytic Reactions

Yeon Joo Cheong, Hye-Young Jang[1,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

There have been many studies on the synthesis of transition metal catalysts with N-heterocyclic carbene (NHC) ligands. Because of its nature, the tight coordination toward metal ions via strong sigma donation capability, the transition metal complexes including NHC ligands show excellent stability. Especially, bidentate NHCs behave like chelating ligands and can provide extra stability and electron-richness on the metal ion. In addition, it is easy to synthesize the modified NHC with various functional groups, such as alcohol, alkoxide, phenoxide, and ether. These additional groups mediate interactions between the ligand and the reactants or between the ligand and the catalyst, which increases the reaction rate and selectivity. In this study, we have made various structurally modified Iridium (III) bis-NHC complexes, which are employed in the conversion of amines to alcohols.

Poster Presentation : **ORGN.P-312**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Reversible Fluorescence Thiol Sensors Targeting Endoplasmic Reticulum

Suhyeon Min, Kihang Choi[1,*]

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

Thiol concentrations in living system are tightly regulated to maintain redox homeostasis, and it is important to be able to monitor the concentration changes in real time to understand the biological functions of thiol compounds. However, most current thiol sensors are based on the irreversible interactions with thiols and not suitable for obtaining reliable data on continuous thiol concentration changes. Our research has previously found that coumarin compounds conjugated with a cyanoacrylamide Michael acceptor react with thiols in a reversible manner and could be used as reversible fluorescence sensors. Based on this finding, we tried to develop a series of fluorescence sensors monitoring thiol concentration changes inside a specific cellular compartment, endoplasmic reticulum (ER). ER is a crucial organelle in eukaryotic cells, and plays important roles in the proper folding and secretion of proteins. ER contains a relatively higher concentration of oxidized glutathione (GSSG), and I would be helpful to measure the concentration of reduced glutathione (GSH) to maintain the cellular homeostasis between GSH and GSSG in ER. To develop ER-specific GSH sensors, various ER targeting moieties were connected to the previously developed coumarin-based reversible thiol sensors. The effect of the linker size between the coumarin fluorophor and the ER targeting moieties was examined and the structure was modified to improve ER retention time and solubility suitable for bioimaging applications. Our study shows that these fluorescent probes can be successfully used to selectively monitor thiol concentration changes in ER.

Poster Presentation : **ORGN.P-313**

Organic Chemistry

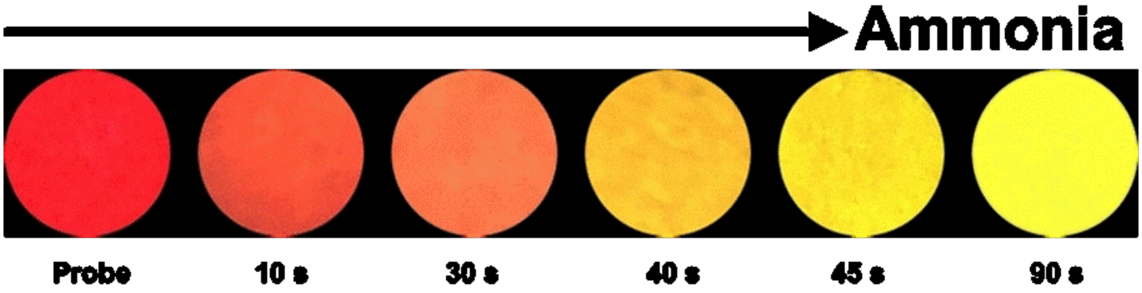
Exhibition Hall 1, FRI 11:00~12:30

A High Sensitive and Selective Fluorescent Probe for the Monitoring of Primary Amines

Sung jin Jeon, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

Ammonia is an important industrial chemical in the synthesis of fertilizer, and one of the most important substances encountered in our daily lives. However, the prolonged exposure to ammonia gas may cause severe problems such as asthma, bronchitis, chronic eye irritation, and dermatitis. Moreover, primary amines such as cadaverine, putrescine, and histamine are considered as important biomarkers for monitoring food quality. Accordingly, it is highly desirable to develop efficient methods for the monitoring of low levels of primary amines in food and industry.In this presentation, we will present a BODIPY-based fluorescent turn-on probe for the sensitive and selective detection of primary amines. Probe displayed a red emission (λ_{em} = 615 nm, φ_F = 0.3) and high photo/chemical stabilities in CH_3CN solution. The reaction of probe with primary amines rapidly trigger highly intense green fluorescent product (λ_{em} = 546 nm, φ_F = 0.8-0.9). The probe also showed high sensitivity (detection limit = 9.8 nM for methyl amine) and high selectivity for primary amines over other amines. Furthermore, a simple and portable paper strip indicator can be successfully applied for the real-time monitoring of ammonia gas leakage and food freshness (**Figure**).



Poster Presentation : **ORGN.P-314**

Organic Chemistry

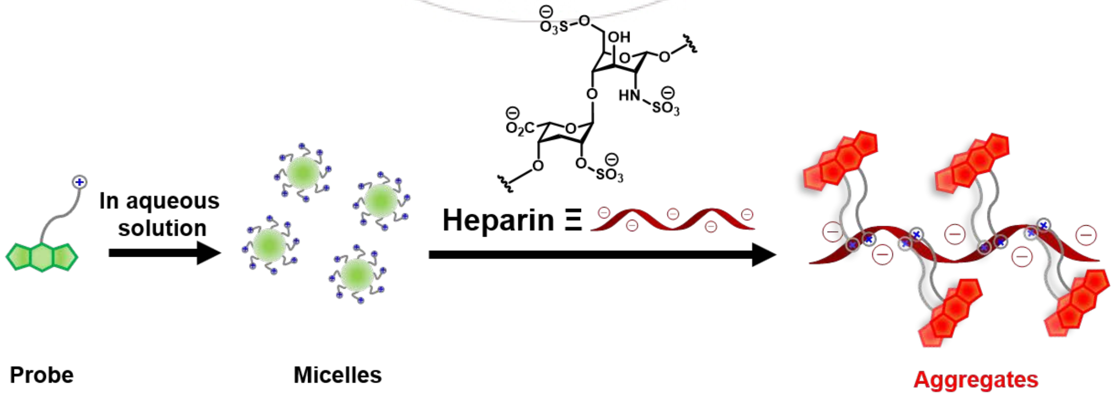
Exhibition Hall 1, FRI 11:00~12:30

A Self-Assembled Micellar Aggregate for the Selective Detection of Heparin.

<u>Dami Kim</u>, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

Heparin is a linear, highly sulfated polysaccharide consisting of disaccharide repeating units. It has a crucial role in various biological processes and tremendous clinical importance as an anticoagulant drug. The sensitive and selective monitoring of the heparin dosage is necessary in clinics.We present a self-assembling fluorophore micelle that functions as a heparin-specific fluorescent turn-on probe. The self-assembled probe micelle displayed only weak green fluorescence in aqueous solution (λ_{em} = 530; Φ_{FL} = 0.018), whereas it would emit bright orange fluorescence (λ_{em} = 585; Φ_{FL} = 0.09) in response to the target analyte through the recognition-driven assembly of the probe and the formation of the probe aggregates on the surface of heparin.We will demonstrate the quantitative detection of heparin in aqueous buffered solution and human serum, as well as the detection of oversulfated chondroitin sulfate (OSCS) in contaminated heparin using enzymatic assay method.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-315**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Direct Allylic C(sp^3)–H Thiolation with Disulfides Enabled by Visible-Light Photoredox Catalysis

Jungwon Kim, Byungjoon Kang, Soon Hyeok Hong[1,*]

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

In spite of the wide utility of allyl sulfides, the direct, catalytic allylic C(sp^3)–H thiolation remains elusive. Here we report a direct allylic C(sp^3)–H thiolation mediated by visible light photoredox catalysis. The use of in-situ generated thiyl radical from disulfide as a hydrogen atom transfer (HAT) reagent and coupling partner enabled selective cleavage of the allylic C(sp^3)–H bond. The undesired hydrothiolation, a prevalent reaction from facile thiyl radical addition to olefins, was prevented by the immediate deprotonation of thiol under basic conditions. A wide range of diaryl disulfides and olefins participated in the reaction, producing allyl sulfides in high efficiency. Mechanistic investigations revealed the participation of the photocatalyst as a redox mediator, which was crucial for the transformation of the allyl radical into an allyl cation and further ionic coupling processes. Based on the mechanistic understanding, limitation in the synthesis of alkyl allyl sulfide was overcome with rationally designed, more electron-deficient unsymmetric disulfide, which makes the desired catalytic cycle operative.

Poster Presentation : **ORGN.P-316**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Highly Active Ruthenium Metathesis Catalysts at Low Temperatures: Unprecedented Ring-Opening Metathesis Polymerization of Cyclopentadiene

Gitaek Song, Jungwon Kim, Chae Eun Heo[1], Hugh I. Kim[1], Soon Hyeok Hong[2,*]

Division of Chemistry, Seoul National University, Korea

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

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

Highly controllable ruthenium catalysts were developed using readily available, versatile N-vinylsulfonamides as the carbene precursors. By facile modulation of the N-vinylsulfonamide ligands, initiation rates of the catalysts were controlled straightforwardly from latent to fast-initiating. Trifluoromethylsulfonyl-based catalysts exhibited considerably high initiation rates even faster than that of the Blechert catalyst, which is one of the fastest-initiating Hoveyda-type catalysts reported so far. To our surprise, the catalyst initiated even at temperatures as low as -60 ℃ and continuously propagated, enabling enthalpically and entropically less-favored ring-opening metathesis polymerizations of low-strained monomers such as cyclopentene. Notably, unprecedented ring-opening metathesis polymerization of cyclopentadiene, a feedstock that is readily obtainable through the steam cracking of naphtha, was realized by performing the polymerization reactions at -40 ℃, which has not been previously achieved due to its low ring strain and facile dimerization even at low temperature (below 0 ℃).

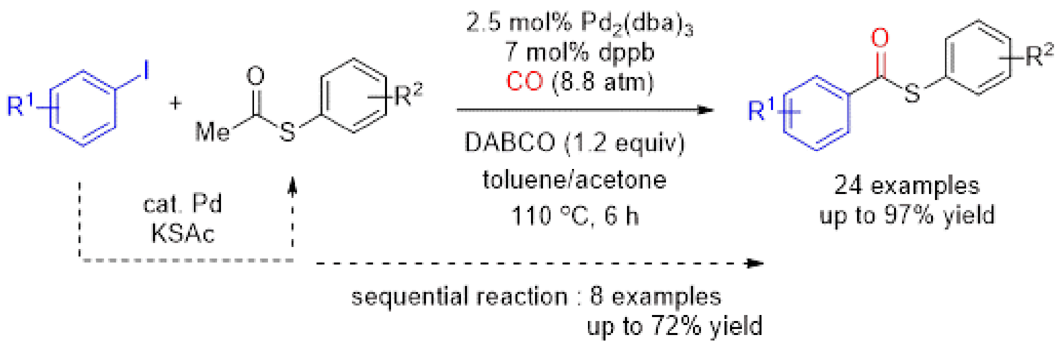
Poster Presentation : **ORGN.P-317**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Pd-Catalyzed Carbonylation of Thioacetates and Aryl Iodide

Yeojin Kim, Sunwoo Lee[*]

Department of Chemistry, Chonnam National University, Korea

Carboxylic ester derivatives including thioesters are one of the most important building blocks in organic synthesis and appear as core group in a number of natural products, agrochemicals, pharmaceuticals, and advanced materials. Many synthetic methods of thioesters have been reported including the palladium-catalyzed carbonylation, decarboxylative coupling of oxocarboxylic acids, oxidative coupling of aldehydes or alcohols and cross-dehydrogenative coupling, however, most of these methods employ thiols as coupling partner. The employment of thiols has several drawbacks such as the requirement of harsh condition as well as the bad odor of thiols. As alternative methods, protected thiols and disulfides have been employed for the formation of thioesters. However, these methods still present some disadvantages such as narrow scope of substrate, high cost, and high reaction temperature. To address these issues, mild and environmentally friendly methods are continuously being sought. We previously reported a palladium-catalyzed coupling reaction of aryl halides and thioacetates for the formation of thioethers.[1] We demonstrated that thioacetates are good coupling partners and provide the desired thioethers in good yields; however, they have not been previously employed in carbonylation reactions. Herein, we employ for the first time thioacetates as sulfur source in the palladium-catalyzed carbonylation of aryl iodides for the formation of thioesters Thioesters were synthesized via palladium-catalyzed carbonylation of thioacetates and aryl iodides. S-Aryl thioacetates coupled with carbon monoxide and aryl iodides to afford the desired S-aryl thioesters in good yields. The reaction showed good functional group tolerance toward fluoro, chloro, ketone, ester, aldehyde, cyano, and nitro groups. The tandem reaction of the direct S-arylation of aryl iodides from potassium thioacetate (KSAc) and subsequent carbonylation of the intermediates S-aryl thioacetates provided S-aryl thioesters in moderate-to-good yields [2].


R1
I
+
O
Me
S
R2
2.5 mol% Pd2(dba)3
7 mol% dppb
CO (8.8 atm)
DABCO (1.2 equiv)
toluene/acetone
110 °C, 6 h
O
S
R1
R2
24 examples
up to 97% yield
cat. Pd
KSAc
sequential reaction : 8 examples
up to 72% yield

Poster Presentation : **ORGN.P-318**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Catalytic C-H Amination for Unsymmetrical Urea Synthesis

Kwangho Yoo, Jooyeon Lee, Hyunjin Kim[1,*], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea
[1]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

Transition metal-catalyzed C-N bond formations are one of the most important bond-forming reactions for organic synthesis and functional group interconversions. Traditionally, N-arylation through N-H activation using Cu and Pd catalysts have been extensively explored (e.g., Buchwald-Hartwig amination reaction). In the last decade, the direct C-H amination reaction using transition metal catalysts have been reported with various organic azides (e.g., acyl-, aryl-, and sulfonyl azides) as N sources.[1] This C-H amination is very efficient and atom economical reactions for C-N bond constructions. In this presentation, we have applied C-H amination reaction for the synthesis of unsymmetrical urea. The C-N bond in urea is successfully created through C-H amination with azides. The derivatization of azides and catalytic condition screenings will be presented along with detail experimental evidences.Reference1. Ryu, J.; Kwak, J.; Shin, K.; Lee, D.; Chang, S. *J. Am. Chem. Soc.* **2013**, *135*, 12861,

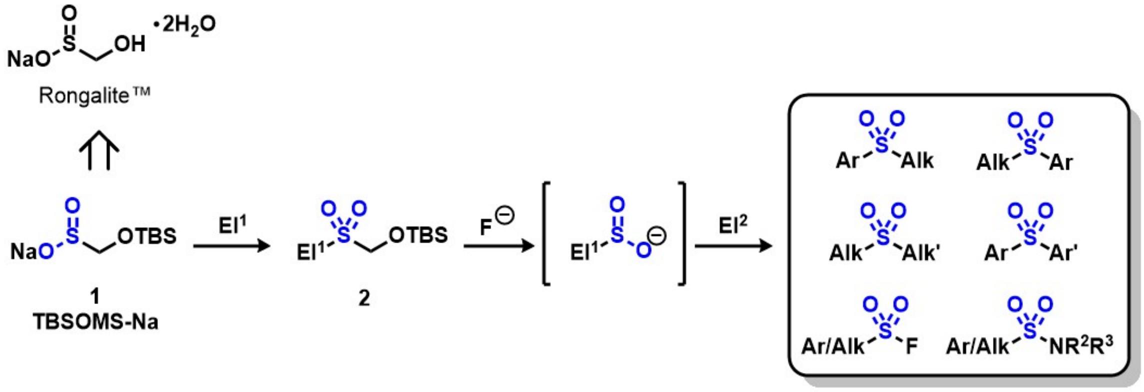
Poster Presentation : **ORGN.P-319**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of sulfones and sulfonyl derivatives using a novel sulfinate

Dae-Kwon Kim, Hyun-Suk Um, Chulbom Lee*

Division of Chemistry, Seoul National University, Korea

Sulfonyl units (-SO$_2$-) occur in many useful organic molecules such as sulfones, sulfonamides and sulfonyl fluorides. Traditionally, their preparation has largely been dependent on oxidizing the sulfur atom in sulfides derived from thiols, which pose handling problems due to their foul odor. In this context sulfur dioxide surrogates have provided useful means for direct introduction of sulfonyl motifs under simple and mild conditions. We explored the use of the novel sulfinate reagent **1** from Rongalite™, previously developed for stereoselective allylic reduction via liberation of sulfur dioxide, for installation of sulfonyl motifs into organic molecules. As a dianion equivalent of sulfur dioxide, sulfoxylate (SO$_2^{2-}$) has the potential for the construction of a wide range of structures by joining with two electrophiles. Recent reports have also disclosed the conceptual demonstration of Rongalite™ or its derivative as a sulfoxylate equivalent. However, the structural variety of accessible sulfones is limited. In contrast, sulfinate **1** is found to be able to react with aryl and alkyl electrophiles to form the stable sulfone intermediate **2**, which can generate a new sulfinate ready for additional alkylation or arylation. Coupling with various aryl electrophiles as well as other functionalization reactions can be carried out with orthogonal unmasking in a single operation. Our studies have shown that sulfinate reagent **1**, a bench-stable white solid, is widely applicable in the synthesis of sulfones and sulfonyl derivatives.


NaO S OH •2H2O
Rongalite™
NaO S OTBS
1
TBSOMS-Na
El1
El1 S OTBS
2
F⊖
El1 S O⊖
El2
Ar S Alk
Alk S Ar
Alk S Alk'
Ar S Ar'
Ar/Alk S F
Ar/Alk S NR2R3

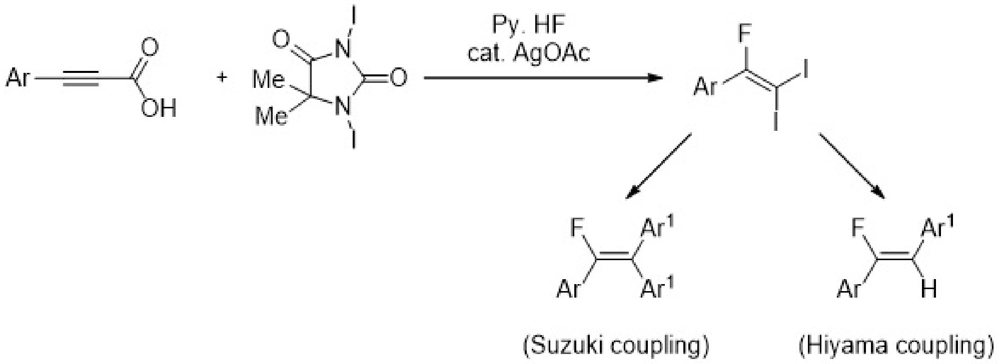
Poster Presentation : **ORGN.P-320**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Silver-Mediated Decarboxylative Halogenation of Alkynoic Acids:Synthesis of Regio- and Stereoselective Fluoroalkenes

Beomseok Ryu, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

A variety of arylalkynoic acids reacted with 1,3-diiodo-5,5-dimethylhydantoin and HF·pyridine in the presence of AgOAc to provide the corresponding 1-fluoro-2,2-diiodovinylarenes in good yields and high regioselectivity. In addition, Pd-catalyzed cross-coupling reaction of 1-fluoro-2,2-diiodovinylarenes afforded diaryl coupling products in the Suzuki reaction and monoaryl coupling products with high stereoselectivity in the Hiyama reaction. It was found that C−Factivated borylation of fluoroalkenes using Pd catalyst afforded the vinylboranes with good yields.



Poster Presentation : **ORGN.P-321**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Enhancing the Performance and Stability of Perovskite Solar Cells by Applying Multifunctional Pt(II) Complex

Eunhye Hwang, Tae-Hyuk Kwon*

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

Perovskite solar cells have been regarded as one of the most promising photovoltaics due to the rapid growth of efficiency from 3.8% to 22.1%.[1] To further improve the power conversion efficiency (PCE), a concept of frequency conversion has been suggested.[2] However, their poor stability against UV light and water still makes it difficult to withstand outdoor conditions. Therefore, it is important to develop a new system that can enhance both the performance and the stability of the perovskite solar cells.

Here, we present a UV-absorbing and hydrophobic Pt(II) complex with high emission quantum efficiency as a dual functional photon down-shifting material for perovskite solar cells. The thin and less-aggregated layer of the compound was fabricated by using the ultrasonic spray deposition method. With this layer, the perovskite solar cells showed the enhanced J_{SC} and PCE, which was corresponding to the increased stability against UV irradiation. Furthermore, the significantly improved humidity-stability for the devices was also achieved by its highly hydrophobic characteristics.

References

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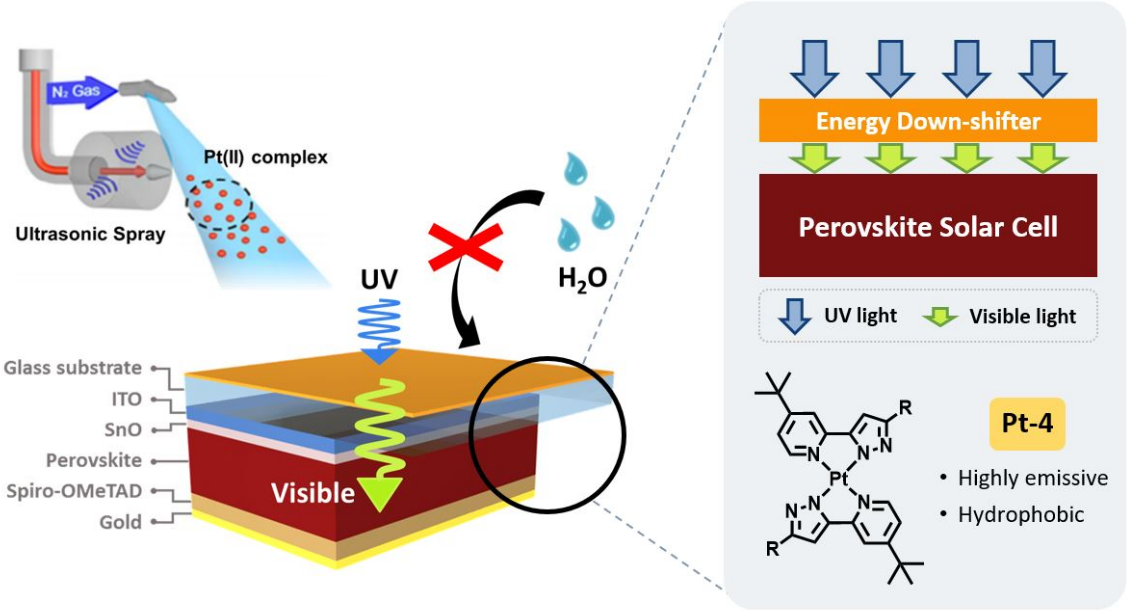
2. Pandey, A.; Kroon, R.E.; Kumar, V.; Swart, H. C. *J. Alloy. Compd.* **2016**, 657, 32-36


N₂ Gas
Pt(II) complex
Ultrasonic Spray
UV
H₂O
Glass substrate
ITO
SnO
Perovskite
Spiro-OMeTAD
Gold
Visible
Energy Down-shifter
Perovskite Solar Cell
UV light
Visible light
R
N
N
N
Pt
N
N
N
R
Pt-4
• Highly emissive
• Hydrophobic

Poster Presentation : **ORGN.P-322**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Palladium-Catalyzed Coupling Reactions of Imine Anion Equivalent of Silyl-Ketimines

Seungjin Jo, Bohee Kim[1], Inji Shin[2,*]

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[1]*Department of Chemistry, Chungnam National University, Korea*
[2]*Department of Fine Chemistry, Seoul National University of Science & Technology, Korea*

The unprecedented palladium-catalyzed cross-coupling reaction of silyl-ketimines with various diaryliodonium salts was studied to give diaryl ketimines. Ketimines are generally prepared from a primary amine and a ketone by the condensation which is sensitive to moistures. However, silyl-ketimines serve as an imine anion equivalents in coupling reactions which can be a practical reversed-polarity alternative to imines.The coupling reactions of silyl-ketimines were optimized using various palladium catalysts, ligands, solvents and additives. With the best reaction conditions, the reaction scopes were investigated with symmetric- and unsymmetric diaryiodonium salts and various silyl-ketimines.

Poster Presentation : **ORGN.P-323**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Conformational analysis of 12/10-helical β-peptides with various acyclic β-amino acids

Jieun KIm, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

β-Peptides having (1R, 2S)-2-aminocyclohexane carboxlic acids((1R,2S)-ACHC) and (1S, 2R)-ACHC with residue alternation form 12/10-helical conformations and the P-helix structure and the M-helix structure equilibrate rapidly in solution. Based on that, we synthesized 12/10-helical β-peptides, in which an acyclic β-amino acid is incorporated between ACHCs and analyzed the change of folding structure through IR, NMR, CD studies. We observed changes in folding structure when incorporating different residues such as β^3-t-butylhomoglycine and β^3-homophenylalanine between ACHCs. This makes it possible to explain the effect of residues on the helical structure, allowing the design of oligomers of the desired structure. It is very interesting to control peptide folding structure and analyze their structure, which is a great help for future foldamer research.

Poster Presentation : **ORGN.P-324**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

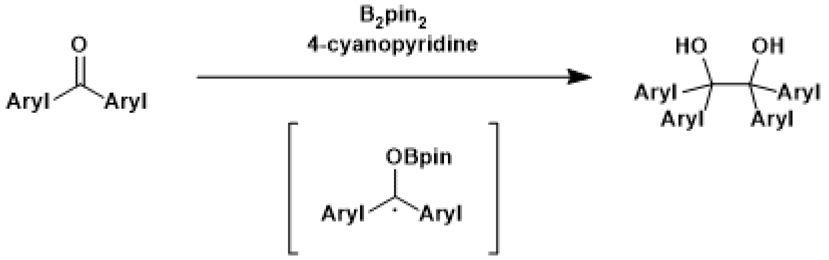
Persistent Boryl Radical-Promoted Pinacol Coupling of Diaryl ketones

Junhyuk Jo, Won-jin Chung*

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

With recent prosper of radical chemistry, the development of chemical reaction utilizing a persistent boryl radical has been being studied actively.[1] The stability and persistency as well as the convenient formation method make the boryl radical useful for application to organic reactions. Employing this reactivity, we developed a pinacol coupling of diaryl ketones which was mostly studied using reductive metals.[2] When a diaryl ketone is heated in the presence of diboron and pyridine, the corresponding diol is produced as a boronate form via the ketyl radical, and upon treatment with an aqueous solution of KHF_2, the desired product can be obtained as free alcohol. The reaction mechanism is proposed on the basis of a well-known reactivity. The pyridine–boryl radical is generated through the homolytic cleavage of the pyridine-diboron complex, and reacts with the diaryl ketone to give the ketyl radical. Finally, the diol is formed through the coupling of the ketyl radicals.

1. a) J. Cao, G. Wang, L. Gao, H. Chen, X. Liu, X. Cheng, S. Li, *Chem. Sci.* **2019**, *10*, 2767–2772. b) J. Cao, G. Wang, L. Gao, X. Cheng, S. Li, *Chem. Sci.* **2018**, *9*, 3664–3671. c) L. Zhang, L. Jiao, *J. Am. Chem. Soc.* **2017**, *139*, 607–610. d) A. Fawcett, J. Pradeilles, Y. Wang, T. Mutsuga, E. L. Myers, V. K. Aggarwal, *Science* **2017**, *357*, 283–286.
2. a) M. Szostak, N. J. Fazakerley, D. Parmar, D. J. Procter, *Chem. Rev.* **2014**, *114*, 5959−6039. b) A. Gansäuer, H. Bluhm *Chem. Rev.* **2000**, *100*, 2771−2788. c) J. E. McMurry, *Chem. Rev.* **1989**, *89*, 1513-1524.


B2pin2
4-cyanopyridine
O
Aryl
Aryl
OBpin
Aryl
Aryl
HO
OH
Aryl
Aryl
Aryl
Aryl

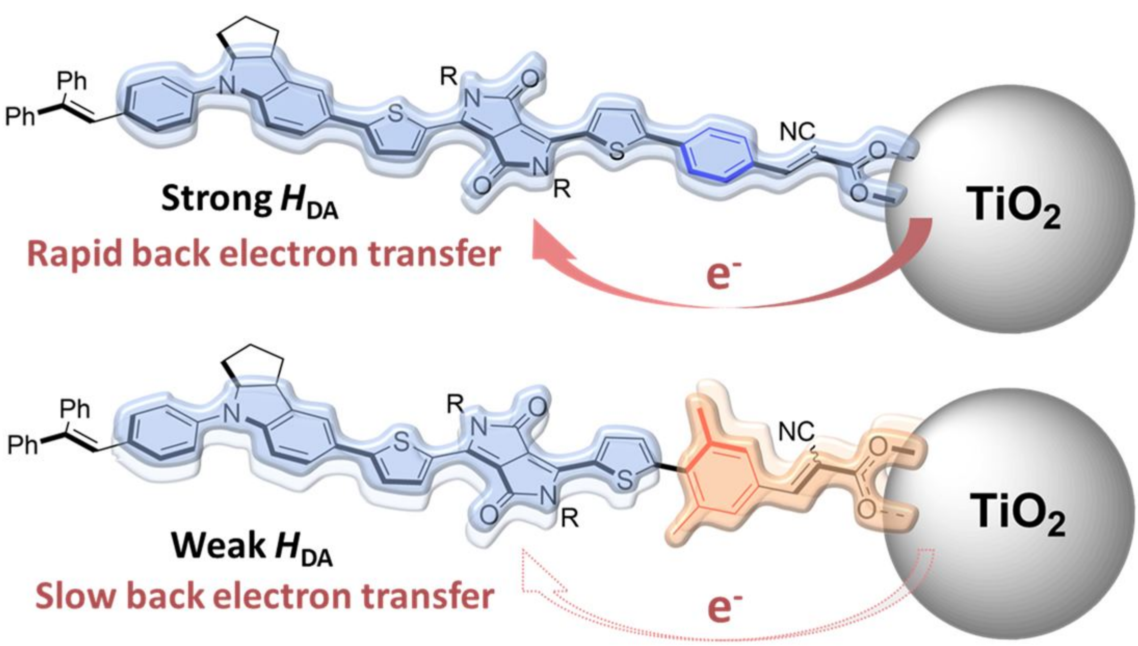
Poster Presentation : **ORGN.P-325**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Control of Electronic Coupling for Retarding Back Electron Transfer in Molecular Solar Cells

Deok-Ho Roh, Tae-Hyuk Kwon[1,*]

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

In molecular solar cells, it is general design strategy of light harvesting materials to have strong electronic coupling (HDA) between electron donor and acceptor for rapid electron transfer and enhancing light harvesting ability. However, strong HDA can promote undesired charge recombination reaction such as back electron transfer from semiconductor to oxidized molecules. Herein, we showed that weak HDA material could enhanced power conversion efficiency (PCE) through efficiently retarding back electron transfer compared with strong HDA materials. We synthesized four sensitizers and controlled magnitude of HDA by geometric torsion of π-spacers (Fig. 1). A planar phenyl spacer (DD-DPP-Ph) that supports strong HDA of 3787 cm-1; and a tolyl spacer (DD-DPP-MP) prevents planarization and decreases HDA of 3314 cm-1; and a twisted xylyl spacer (DD-DPP-DMP) fully distorts π-conjugation and have weak HDA of 984 cm-1 without a significant change in absorption spectra. In device results, the weak HDA of DD-DPP-DMP showed ca. 36% enhanced PCE (8.6%) with high JSC (17.71 mA/cm2) owing to reduced back electron transfer compared with those of the strong HDA DD-DPP-Ph. In addition, we introduced bulky donor unit into weak HDA of sensitizer (bTPA-DPP-DMP) to maximize PCE. As a result, bTPA-DPP-DMP gave a PCE of 9.3% and a 10% PCE are achieved using co-sensitization with D35. Collectively, the results showed that a strong HDA induced rapid back electron transfer, resulting poor device performances. In contrast, a weak HDA efficiently retarded back electron transfer, and enhanced PCE. These findings should be considered for designing materials for molecular solar cells


Ph
Ph
N
R
O
S
N
R
O
S
NC
O
O
TiO$_2$
Strong H_{DA}
Rapid back electron transfer
e$^-$
Ph
Ph
N
R
O
S
N
R
O
S
NC
O
O
TiO$_2$
Weak H_{DA}
Slow back electron transfer
e$^-$

Poster Presentation : **ORGN.P-326**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Cobalt-Catalyzed C–F Bond Silylation of Aryl Fluorides

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Department of Chemistry, Pohang University of Science and Technology, Korea
[1]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Korea*

Fluorine atom can be found in a variety of organic molecules such as pharmaceuticals, agrochemicals, and polymeric materials.[1] In line with an importance of fluorinated compounds, there have been significant advances on C−F bond formation for the past decades.[2] However, unlike 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 2018, defluorosilylation of aryl fluorides has been developed for the first time by Shibata group[3] and in this year, Martin[4] and Studer[5] group reported other defluorosilylation systems. However, highly activated silylating reagents were necessary and only one type of silyl functional group could be applied in previously developed systems. In order to overcome such limitation, we have been explored Co-based catalysis and here we present cotalt-catalyzed unactivated aryl C−F bond silylation. This reaction can be set up under aerobic condition and do not require a presynthesized organometallic complex. Furthermore, different types of silylating reagents can be used in this system. A mild and practical Co-catalyzed silylation of various fluoroarenes enables a new reaction strategy in synthetic chemistry.Reference(1) J. Wang, M. Sánchez-Roselló, J. L. Aceña, C. del Pozo, A. E. Sorochinsky, S. Fustero, V. A. Soloshonok, H. Liu, *Chem. Rev.* **2014**, *114*, 2432.(2) T. Liang, C. Neumann, T. Ritter, *Angew. Chem. Int. Ed.* **2013**, *52*, 8214.(3) B. Cui, S. Jia, E. Tokunaga, N. Shibata, *Nature Communications* **2018**, *9*, 4393.(4) X. Liu, C. Zarate, R. Martin, *Angew. Chem. Int. Ed.* **2019**, *58*, 2064.(5) S. Mallick, P. Xu, E.Würthwein, A. Studer, *Angew. Chem. Int. Ed.* **2019**, *58*, 283.

Poster Presentation : **ORGN.P-327**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Biological Investigation of Novel Hybrid Molecules for Anti-inflammatory Activity

Ju Mi Lee, Jeong Tae Lee*

Chemistry, Hallym University, Korea

Recent scientific databases show the increasing interest in the development of compounds which are able to address multiple targets. In this study, synthesis and biological evaluation of novel hybrid molecules was described. Anti-inflammatory and antihistamine drug candidates were utilized as building blocks to generate the hybrid molecules. Salicylic acid, well known as an anti-inflammatory agent by inhibiting nuclear factor kappa B (NF-κB), was exploited in this examination. The inhibitory effect of the synthesized hybrid compounds on NO production was investigated as an indicator of anti-inflammatory activity.

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Poster Presentation : **ORGN.P-328**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Resveratrol Analogues having Nitrogen Heterocycles : Syntheses and Biological Activity Evaluation

Lee Seul Park, Jeong Tae Lee*

Chemistry, Hallym University, Korea

Nitrogen containing heterocycles are among the most remarkable structural components of pharmaceuticals. Resveratrol (3,5,4'-*trans*-trihydroxystilbene) is a nutraceutical with diverse therapeutic effects such as antioxidant, anti-inflammatory and anticancer activity. To improve its biological activity, nitrogen containing π-expanded resveratrol analogues were synthesized and explored their antioxidant and anti-inflammatory activity.

Poster Presentation : **ORGN.P-329**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Resveratrol Derivatives Containing Heteroatoms

Hyeongryeol Woo, Jeong Tae Lee*

Chemistry, Hallym University, Korea

Resveratrol (3,5,4'-*trans*-trihydroxystilbene) is a well-known natural product in view of its exciting pharmacological potential including cardiovascular protective, antiplatelet, antioxidant, antiinflammatory, blood glucose-lowering and anticancer activities, hence it exhibits a complex mode of action. However, in most of the studies, the major hurdle was its poor bioavailability. Thus, this work was aimed to improve its activity by the synthesis of π-system extended resveratrol derivatives having heteroatoms. We prepared a set of derivatives containing heteroatoms and their regioisomers to discern how the position of heterotoms in extended resveratrol affect antioxidant effects.

Poster Presentation : **ORGN.P-330**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

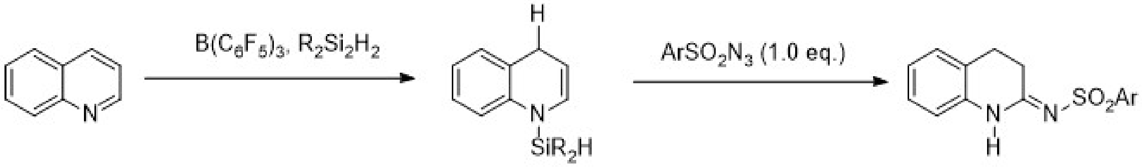
Synthesis of cyclic amidines from quinolines via cascade hydrosilylation and [2+3] cycloaddition

Vinh Do Cao, Seewon Joung*

Department of Chemistry, Mokpo National University, Korea

Amidine is one of the fundamental functional group in organic synthesis and pharmaceutical molecules. In particular, cyclic amidines are versatile structural motifs in various natural and synthetic compounds with wide range of bioactivities. As a result, development of synthetic route to cyclic amidines has been investigated extensively. Among them, [2+3] cycloaddition of azide and enamine has garnered special attention since the resulting triazole intermediate can be utilized for various reaction pathways. On the other hand, Borane catalyzed hydrosilylation of N-heterocycles had been developed by Chang and coworkers. Mechanistic study revealed that there is a partially reduced endocyclic enamine intermediate that can be used as versatile building block.

Herein, a new synthetic route to cyclic amidines from readily available quinolines has been developed. Activation of the stable quinoline with borane catalyzed monohydrosilylation gave us the versatile silyl enamine intermediate. Subsequent addition of organic azides to the intermediate resulted in unique class of cyclic amidines, 3,4-dihydroquinolinimines.



Poster Presentation : **ORGN.P-331**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Phenolic Amides from the Leaves of *Nicotiana tabacum* and Their Derivatives

Kongara Damodar, Jeong Tae Lee*

Chemistry, Hallym University, Korea

The therapeutic effects of phenolic amides has attracted much attention and they have been acknowledged as having interesting medicinal properties, such as anti-inflammatory, antiviral, anticancer and anti-coagulant activities. *Nicotiana tabacum*, tobacco, is smoked or chewed as a drug for its mild stimulant effects and also used as an insecticide, anesthetic, diaphoretic, sedative, and emetic agent in Chinese folklore medicines. This study describes the first synthesis of phenolic amides **1–3** isolated from *N. tabacum* and their derivatives **4–12**.

Poster Presentation : **ORGN.P-332**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthetic Investigation of Disubstituted Benzene Derivatives Containing Aromatic Imides

Sung Sik Kim

Department of Chemistry, Chonbuk National University, Korea

Several types of benzene derivatives were synthesized for the study of intra- and intermolecular electron transfer processes of aromatic imides. Target molecules contain 1,8-phthalimide, naphthalenetetracarboxylic diimide, and perylene monoimide at the central benzene ring. Target molecule 1 was synthesized from naphthalenetetracarboxylic dianhydride as the starting material. Naphthalene monoimide intermediate was reacted with phenylenediamine in N,N-dimethylformamide (DMF) to give an aminobenzene derivative having naphthalene diimide. This diimide was reacted with phthalic anhydride in DMF to give the target molecule 1 having naphthalene diimide and phthalimide. Target molecule 2 having naphthalenetetracarboxylic diimide and naphthalene monoimide was prepared from 1,8-naphthalic anhydride as the starting material. The anhydride was reacted with 1,3-diaminobenzene in DMF to give an aminobenene derivative containing 1,8-naphthalimide, which was reacted with naphthalene anhydride imide to give the target molecule 2, a benzene derivative containing naphthalene diimide and naphthalene monoimide. The target molecule 3, a benzene derivative containing naphthalenetetracarboxylic diimide and perylene monoimide was prepared from perylenetetracarboxylic dianhydride as the starting material. The dianhydride was reacted with 2,6-diisopropylaniline in imidazole/zinc acetate monohydrate to give perylene monoimide, which was converted into the corresponding monoanhydride by using KOH/t-BuOH and HCl. The monoanhydride was reacted with 1,3-diaminobenzene in DMF to give a benzene derivative having perylene monoimide, which was finally reacted with naphthalene anhydride imide in DMF to give the target molecule 3, a benzene derivative having naphthalene diimide and perylene monoimide. Synthesis of another types of benzene derivatives was also described in this study.

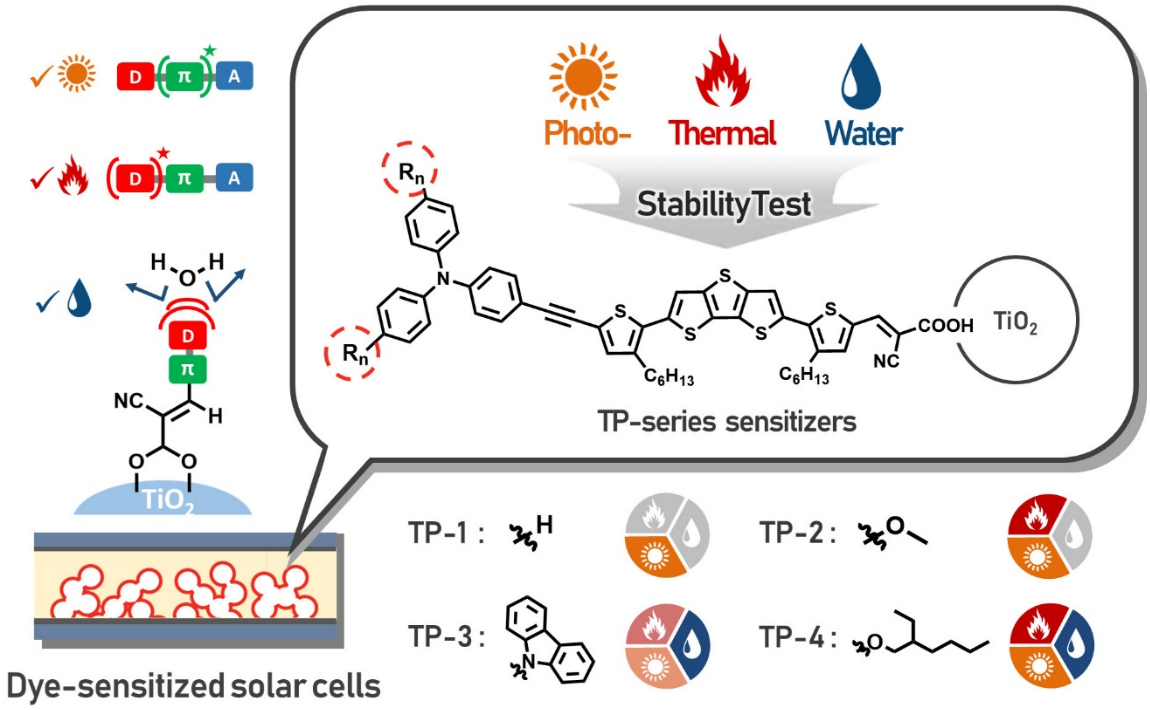
Poster Presentation : **ORGN.P-333**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Molecular Design Strategy toward Robust Organic Dyes in Thin-Film Photoanodes

Jun-Hyeok Park, Wanghyo Kim[1], Deok-Ho Roh[2], Tae-Hyuk Kwon[3,*]

Division of Natural Sciences, Ulsan National Institute of Science and Technology, Korea
[1]*Ulsan National Institute of Science and Technology, Korea*
[2]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*
[3]*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*

Dye-sensitized solar cells (DSSCs) have attracted attentions because of application to building integrated photo voltaic (BIPV) system. It has several advantages, especially very high efficiency at low illumination. However, there have been still stability issues and molecular strategy for rigid stability have not been systemically suggested. In this work, we suggested functional groups on the donor moiety and reveal relationship between molecular structure and degradation pathways divided into photo/thermal/water environmental factors. In this work, we introduced TP-series sensitizers which have basically π-conjugated bridge unit as dithieno[3,2-b:2',3'-d]thiophene(DTT) which planarity and strong stability. In detailed, four sensitizers have different functional groups on donors and we found that functional groups in donor moiety affect PCE and alkoxy functional groups (TP-2 and 4) is more effective to obtain high performance, because of increasing donating ability and rapid Intermolecular Charge Transfer (ICT). Furthermore, they show good thermal and light stability because of stabilization excited or oxidized state by donating effect. However, in case of TP-3, it exhibited weak thermal and light stability because 3,6-position of carbazole were easily oxidized by external energy, but achieved the highest water stability presumably by the strong hydrophobicity of carbazole group. In contrast, TP-2 showed the lowest water stability because of high hydrophilicity. Therefore, TP-4 with a 2-ethylhexyloxy group was designed and synthesized for protecting oxygen on alkoxy group. As a result, TP-4 achieved high stabilities in terms of thermal, light and water stability and a PCE as high as 8.86% due to the strong electron donating ability as shown in the methoxy group of TP-2.


D
π
A
H
O
H
NC
H
O
O
TiO2
Photo-
Thermal
Water
Stability Test
Rn
Rn
N
S
S
S
S
S
C6H13
C6H13
COOH
NC
TiO2
TP-series sensitizers
TP-1 :
H
TP-2 :
O
TP-3 :
N
TP-4 :
O
Dye-sensitized solar cells

Poster Presentation : **ORGN.P-334**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Theoretical Study on the Effects of Various Counter Cations in Alkylation of Ambident Enolates Ionpairs

Jiin Oh, Keepyung Nahm[*]

Department of Chemistry, Yeungnam University, Korea

We calculated the alkylation of ambident enolate ion pairs, with various counter cations. And we compared (Z)- and (E)-enolates in the alkylation. Based on this calculation, the TS energy for the alkylation with counter cations was correlated.

Poster Presentation : **ORGN.P-335**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Polyphenols for the Synthesis of Cyclic Carbonates at Room Temperature and Atmospheric CO2

Jieun Lee, Youngjo Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

The coupling reaction of CO2 and epoxides yielding cyclic carbonates, used as polar aprotic solvents, electrolytes for lithium–ion batteries, monomers for polymerizations, and pharmaceutical intermediates, is one of the most active research areas of CO2 conversion due to its atom economy (no side products) and broad applicability. Even though organocatalysts have many advantages in terms of cost, toxicity, and accessibility, compared to metal-based catalysts, they generally require harsh reaction conditions such as high temperatures (> 100 °C), high CO2 pressures (> 10 bar), and high catalyst loadings (> 5 mol %) for the efficient conversion. To date, several active organocatalysts for this coupling reaction under mild conditions have been reported in the literature; however, the development of efficient organocatalysts capable of operating at ambient temperature and atmospheric CO2 pressure is clearly a difficult task and just a few examples are known. The detailed synthesis, characterization, and catalytic activities of new polyphenol-based organic compounds will be discussed.

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Poster Presentation : **ORGN.P-336**

Organic Chemistry

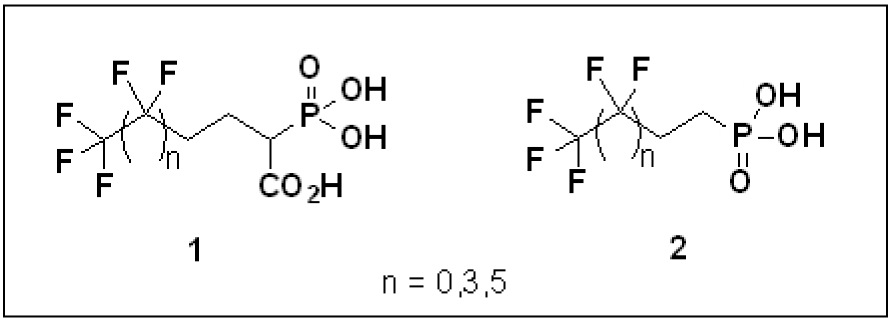
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of fluorinated-2-phosphonobutanoic acid and fluorinated-ethylphosphonic acid

Kyung-min Choi, Yeonsu Choi, Jihye Park, Dong-Soo Shin*

Department of Chemistry, Changwon National University, Korea

In this study, as PFOA alternatives, compound 1 and 2 were designed and synthesized. Fluorinated-2-phosphonobutanoic acid (1) was synthesized in two steps using triethyl phosphanoacetate and fluoroethyl iodide and fluorinated-ethylphosphonic acid (2) was synthesized in two steps and will be presented the detailed synthesis methods.



Poster Presentation : **ORGN.P-337**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Properties of Structurally Different Pyrazine Derivatives and Investigation of Their Optical, Thermal and Electrochemical Properties for Optoelectronic Applications

Dong Jin Park, Hyungha Park, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Pyrazine is an important molecular scaffold employed in organic optoelectronic materials. Here we describe the synthesis and optoelectronic characterization of pyrazine derivatives decorated with donor and acceptor moieties. Synthetic method has been developed for the preparation of pyrazine derivatives by employing palladium catalysed Suzuki coupling reactions under microwave conditions. Pyrazine derived structural isomers has been prepared with different donor and acceptor groups. They show different optical electrochemical properties. A comprehensive study of the optical properties, and molecular packing of the synthesized compounds was carried out. The optical, thermal and electrochemical properties of the materials are analysed and the results are supported with the DFT calculations.

Poster Presentation : **ORGN.P-338**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Comparative Study on Photophysical Properties of Methyl Salicylate Derivatives

Miyeon Yoon, Nam Gi Cho[1], Intae Kim*

Department of Chemistry, Kwangwoon University, Korea
[1]*chemistry, Kwangwoon university, Korea*

Three different S, N, Se-modified methyl salicylate derivatives, methyl 2-hydroxy-4-(pyridin-2-yl)benzoate(MHPB), methyl 2-hydroxy-4-(thiophen-2-yl)benzoate(MHTB) and methyl 2-hydroxy-4-(selenophen-2-yl)benzoate(MHSB) have been synthesized and their photophysical properties are examined in dichloromethane. The three derivatives produce absorption spectra with different shapes spanning over 260-370 nm region. In this work, we have compared with the characteristic emission features of the three derivatives. For MHPB, two emission bands are observed with relatively strong intensities. However, for MHTB the intensity of the blue emission is reduced and for MHSB the emission is quenched. Also, we have calculated quantum yields and observed lifetimes of the three derivatives. Through this work, we can study comparative photophysical properties of the three derivatives, and it is expected to widen the application of methyl salicylate derivatives.

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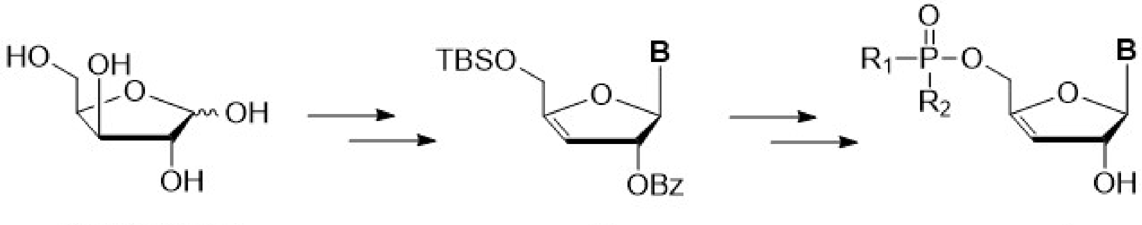
Poster Presentation : **ORGN.P-339**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of evaluation of 3′, 4′-dihydronucleosides and their phosphoramidate prodrugs

JiSu Kim, SeMyeong Choi[1], Jong Hyun Cho[*]

Department of Medicinal Biotechnology, Dong-A University, Korea
[1]*Department of Health science, Dong-A University, Korea*

Ji Su Kim,[a] Se Myeong Choi,[a] Jong Hyun Cho[a*][a]*Department of Medicinal Biotechnology, College of Health Science, Dong-A University, Busan 49315, South Koreae-mail:jhcho1@dau.ac.kr***Abstract**A naturally occurring 3’-deoxy-3′,4′-dihydro-cytidine triphosphate (ddhCTP) in mammalian cell, showed a broad spectrum of antiviral activity as a chain terminator for RNA-dependent RNA polymerases (RdRps) against Flavivirus genus.[1] On the basis of its sugar-ring scaffold, a series of 3-dexoy-3′,4′-dihydroribonucleoside derivatives (**2**) were successfully synthesized by utilizing 1,2-elemination reaction with mild organic bases from D-xylose. As the key step, the 3’-sulfonylated D-xylonucleoside (A, G, C, T, U) derivatives were treated with organic bases and removal of silyl and benzoyl groups to give their corresponding 3’-deoxy-3′,4′-dihydro-ribonucleosides (**2**) in quantitative yield. Finally, the reaction of 3’-deoxy-3′,4′-dihydronucleosides (**2**) with a phosphoramidate derivative (**3**) provided their ProTides in good yield.**Figure 1. References**1) Gizzi, A.S.; Grove, T.L.; Arnold, J.J.; Jose, J.; Jangra, R.K.; Garforth, S.J.; Du, Q.; Cahill, S.M.; Dulyaninova, N.G.; Love, J.D.; Chandran, K.; Bresnick, A.R.; Cameron, C.E.; Almo, S.C. *Nature*. **2018**, *558*, 610–614.2) Liu, Q.; Cai, X.; Yang, D.; Chen, Y.; Wang, Y.; Shao, L.; Wang, M.W. *Bioorg. Med. Chem*. **2017**, *25*, 4579-45943) Saito, Y.; Nyilas, A.; A, L.; Agrofoglio. *Carbohydrate Research*. **2001**, *331*, 83–904) Vorbrüggen, H.; Krolikiewicz, K.; Bennua, B. *Chem. Ber. Recl*. **1981**, *114*, 1234-1255



D-Xylose (1) **2** **3**

Poster Presentation : **ORGN.P-340**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Alkylative Aziridine Ring Openings

Taehwan Yu, Won Koo Lee[1], Hyun-Joon Ha[2,*]

Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry, Sogang University, Korea*
[2]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Aziridine, a nitrogen-containing three membered ring, has similar high ring strains as oxirane and cyclopropane. However, non-activated aziridine bearing electron donating group at the ring nitrogen is stable and inert toward almost all nucleophiles, which should be activated properly as aziridinium ion or its equivalent prior to ring opening reaction.This reactivity provides an opportunity to introduce another functional group into the nitrogen during activation of aziridine ring. We succeeded alkylation of the ring-nitrogen including methyl, ethyl and allyl to give rise to alkylated acyclic amines after opening the aziridine ring.

Poster Presentation : **ORGN.P-341**

Organic Chemistry

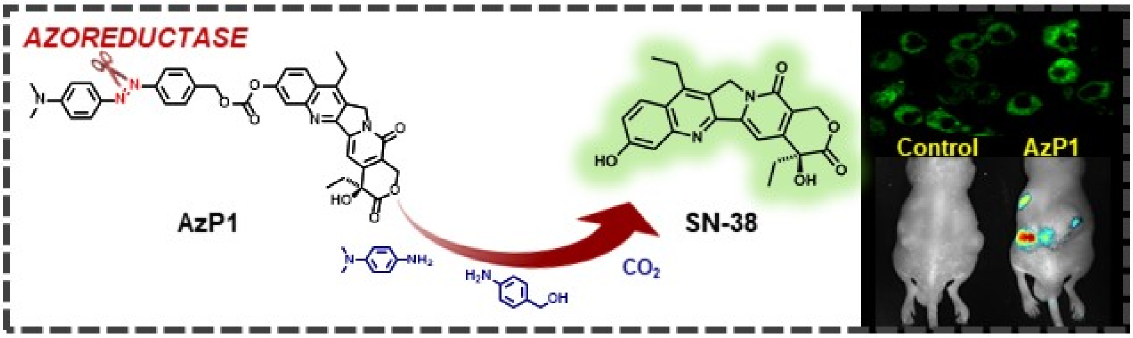
Exhibition Hall 1, FRI 11:00~12:30

Drug activation and tumor imaging under hypoxic conditions with azo-based small molecule

Wonseok Choi, Hyeong Seok Kim, Jinwoo Shin, Subin Son, Ji Hyeon Kim, Myung Sun Ji, Jusung Ahn, Jongseung Kim*

Department of Chemistry, Korea University, Korea

We report herein, an azo-derivative (AzP1) of FDA approved antineoplastic drug SN-38 (irinotecan analogue) as a theranostic agent with a potential for both tumor hypoxia-specific activation and therapy. The theranostic AzP1 was found to be stable within a biologically relevant pH scale and was chemically inert towards other competitive biological analytes. However, upon treatment with rat-liver microsomes, AzP1 showed a self-calibrated fluorescence enhancement at λem=560 nm. The cytotoxicity profile of AzP1 was tested in various cancer lines. Under hypoxic conditions, prodrug AzP1 exhibited activation to release the parent drug (SN-38) and enhanced cytotoxicity in cancer cells with concomitant fluorescence enhancement at 560 nm, which served to monitor both the drug activation and tracing purposes. The therapeutic potential of AzP1 for both tumor-specific activation and suppression of tumor weights was validated in xenograft mouse model. Collectively, the synthetic ease and hypoxia-sensitive activation along with promising therapeutic properties highlight the potential of theranostic AzPI in future cancer treatment programs.



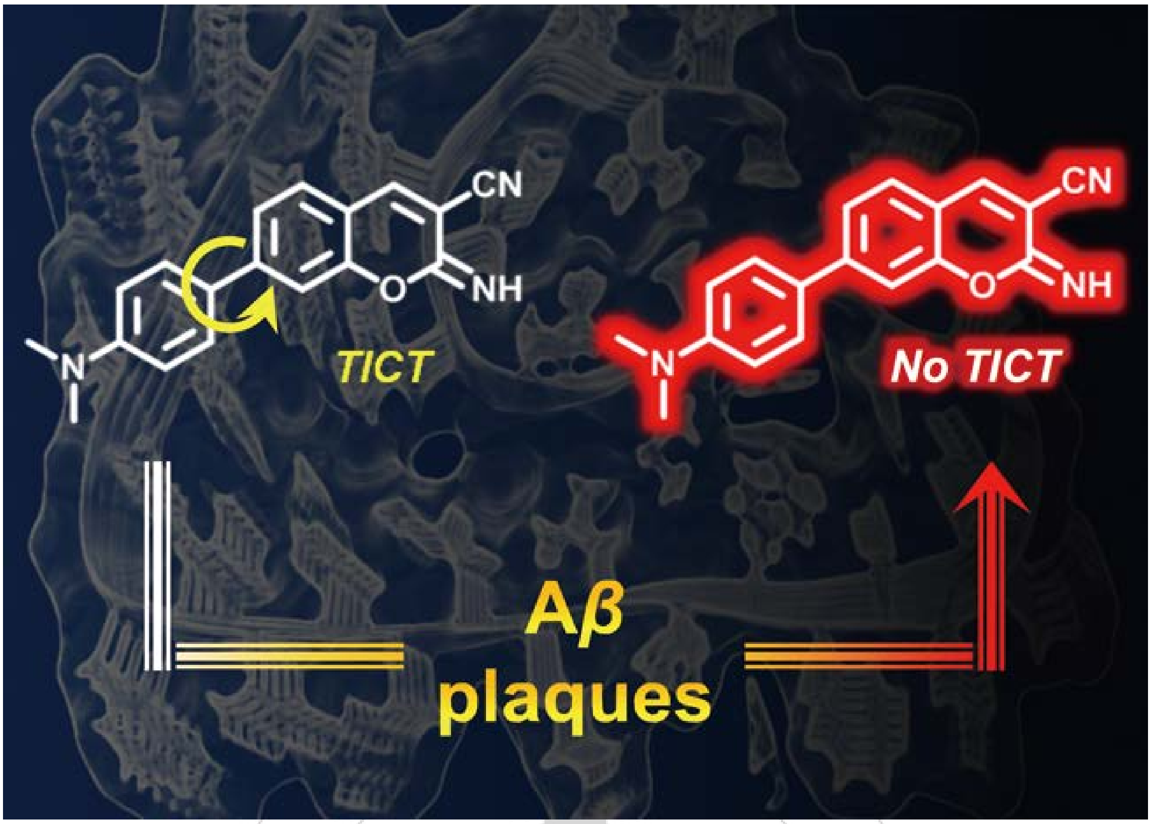
Poster Presentation : **ORGN.P-342**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Minimizing Background Fluorescence in Brightly Emissive Two-Photon β-Amyloid Dyes

Jinwoo Shin, Jiseon Kim, Jusung Ahn, Hyeong Seok Kim, Ji Hyeon Kim, Subin Son, Myung Sun Ji, Wonseok Choi, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Alzheimer's disease (AD) is one of the most progressive neurodegenerative disease eventually leading to fatality. As the most abundant proteinaceous deposit in the brains of AD patients, β-Amyloid (Aβ) has been the subject of intensive research efforts. Fluorescent labeling of Aβ plaques has been the most widely used method for the investigation of the disease in animal models. Two-photon spectroscopy offers many advantages, such as a higher spatial resolution and a deeper penetration depth. The latest two-photon Aβ fluorophores, such as MethoxyX-04 and IBC2, have often adopted a rigidified molecular framework to maximize the two-photon properties and have been demonstrated to readily cross the BBB and label Aβ plaques in vivo. However, generally these rigid fluorophores exhibit a considerable amount of off-target fluorescence. In the current work, we set out to investigate the two-photon properties of an imino-coumarin dye, endowed with a rotatable bond to minimize fluorescence in the absence of Aβ plaques. The fluorescence of the dye was found to be fully quenched in aqueous solutions, whereas bright fluorescence was observed in the presence of Aβ plaques. The behavior of the dye was rationalized using a theoretical approach, demonstrating the involvement of a twisted-intramolecular charge transfer (TICT) state in polar solvents. Docking studies demonstrated a high-affinity binding pocket adjacent Phe20, along the fibril axis. In vivo two-photon imaging of distribution of Aβ plaques using IRI-1 and Methoxy-X04 demonstrated the rapid accumulation of the dye in the brain of transgenic mouse (5XFAD, 11-month-old), following intraperitoneal injection and labeling of Aβ plaques in the cortical regions.


CN
NH
O
N
TICT
CN
NH
O
N
No TICT
Aβ
plaques

Poster Presentation : **ORGN.P-343**

Organic Chemistry

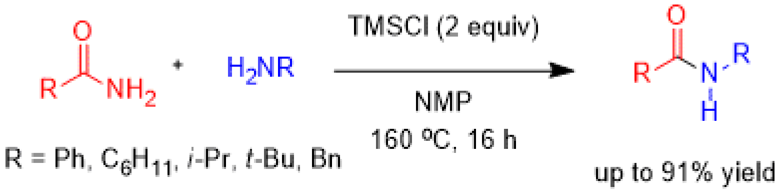
Exhibition Hall 1, FRI 11:00~12:30

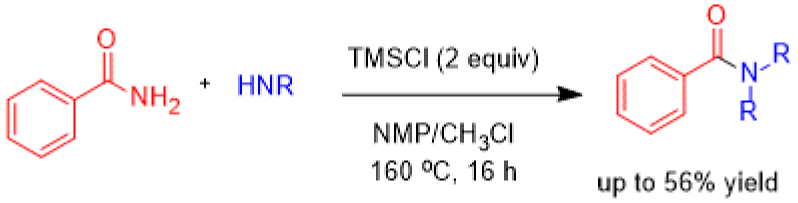
Transamidation of Primary Amides by using Trimethylsilyl Chloride

Eunkyeong Seo, Sunwoo Lee[1,*]

Chemitry, Chonnam National University, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*

The amide functional group is one of the most important moieties in nature because it is the backbone of proteins and peptides. Amide-containing compounds have received much attention because they are widely used for the synthesis of bioactive molecules in pharmaceutical and agricultural chemistry, and are also of great relevance to material science. Therefore, synthesis methods for the preparation of the amide functional group have been widely developed. Transamidation of amides with amines has recently gained considerable momentum, although the activation of the C-N bonds of amides is hardly achieved, because of the ready availability of amines and straightforward tools. A number of efficient methods for this modern strategy have been intensively developed for decades. Although it is known that the transamidation of secondary amides is a challenging project, and that the transamidation of primary amides is relatively more studied, the latter still has some hurdles to overcome. Recently, we found that TMSCl activated secondary amides in nickel-catalyzed transamidation reactions, and we reported the direct transamidation of secondary amides with primary and secondary amine. Based on these results, we envisioned that TMSCl might activate primary amides in transamidation reactions without any metal catalyst. To the best of our knowledge, TMSCl-mediated transamidations have not been reported. Herein, we report metal-free transamidation of primary amides using TMSCl.We developed metal-free transamidation of primary amides. TMSCl acted as the activator in transamidation. In the presence of TMSCl, primary amides reacted with primary amines to yield transamidated secondary amides in NMP solvent. The transamidation of benzamide with secondary amines for the formation of tertiary amides succeeds in NMP/CH_3Cl solvent.


O
R
NH$_2$
+
H$_2$NR
R = Ph, C$_6$H$_{11}$, *i*-Pr, *t*-Bu, Bn
TMSCl (2 equiv)
NMP
160 ºC, 16 h
O
R
N
R
H
up to 91% yield


O
NH$_2$
+
HNR
TMSCl (2 equiv)
NMP/CH$_3$Cl
160 ºC, 16 h
O
N
R
R
up to 56% yield

Poster Presentation : **ORGN.P-344**

Organic Chemistry

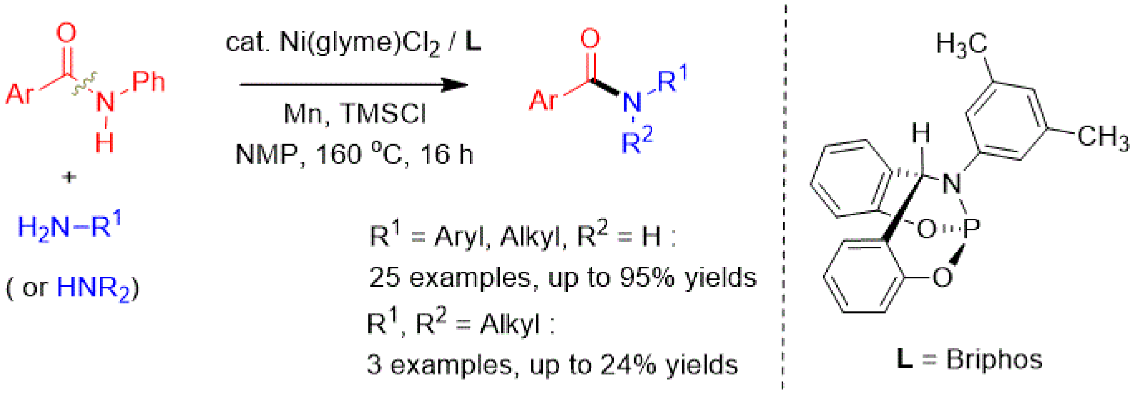
Exhibition Hall 1, FRI 11:00~12:30

Ni-Catalyzed Transamidation of Secondary Amides by using Trimethylsilyl Chloride

Dahyeon Yang, Sunwoo Lee[1,*]

Chemistry department, Chonnam National University, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*

The amide functionality is one of the key structural motifs found in biological compounds such as peptides, proteins, and alkaloids as well as widely used to prepare agrochemicals, pharmaceuticals, polymers, and materials. A promising solution to activate the amides is the transition metal catalyzed C-N bond activation. For the last decade, a variety of synthetic methods have been developed to convert amides to other amides, esters, and ketones. However, the efficient methods were developed with tertiary amides while secondary amides are considered to be challenging. Two-step approaches were recently developed with a concept that the secondary amides were first converted to activating tertiary amides with tosyl or tert-butyloxycarbonyl (Boc) groups by using tosyl chloride or di-tert-butyl carbonate (Boc2O), respectively. The N-functionalized amides were then allowed to react with amines to provide the corresponding secondary amides in good yields. Garg and Szostak groups developed catalytic systems with nickel and palladium, respectively. Another method to prepare N-Boc-activated amides was reported by Hu group, employing nitroarenes as amine surrogates and nickel-catalyzed reductive transamidation. Because the two step approaches still require a preparation step for introducing activating group, it is highly desirable to develop the direct transamidation of the secondary amides. Herein, we report the direct transamidation of secondary amines. The direct nickel-catalyzed transamidation was significantly improved in the presence of our π-acidic briphos ligand and trimethylsilyl chloride (TMSCl). The employment of TMSCl does not require the preparation step of activating tertiary amide from the secondary amide. It is believed that TMSCl activated the aniline derivatives through the formation of the corresponding bis(trimethylsilyl)anilines. The reaction of secondary amide and anilines smoothly proceeded to afford the transamidation product with moderate to good yields. Aniline derivatives having electron donating group showed higher yields than those having electron withdrawing group.



R^1 = Aryl, Alkyl, R^2 = H :
25 examples, up to 95% yields
R^1, R^2 = Alkyl :
3 examples, up to 24% yields

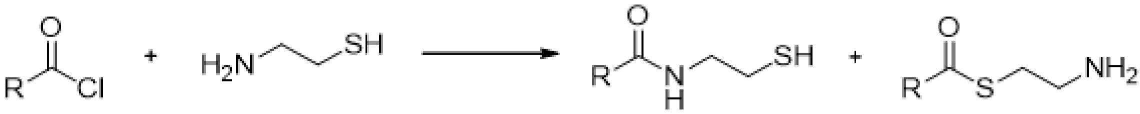
Poster Presentation : **ORGN.P-345**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

The Chemoselectivity between S- and N-Acylation of β-mercaptoamine with Acid Chloride Depending on Reaction Conditions

Myeonghwan Shin, **Chuljin Ahn**[1,*]

Department of biology and chemistry, Changwon National University, Korea
[1]*Department of Biology and Chemistry, Changwon National University, Korea*

The chemoselectivity is important to control functionalization in a molecule. In this research, we investigated the selectivity between S-acylation and N-acylation depending on reaction conditions with β-mercaptoamine and acid chloride.



Poster Presentation : **ORGN.P-346**

Organic Chemistry

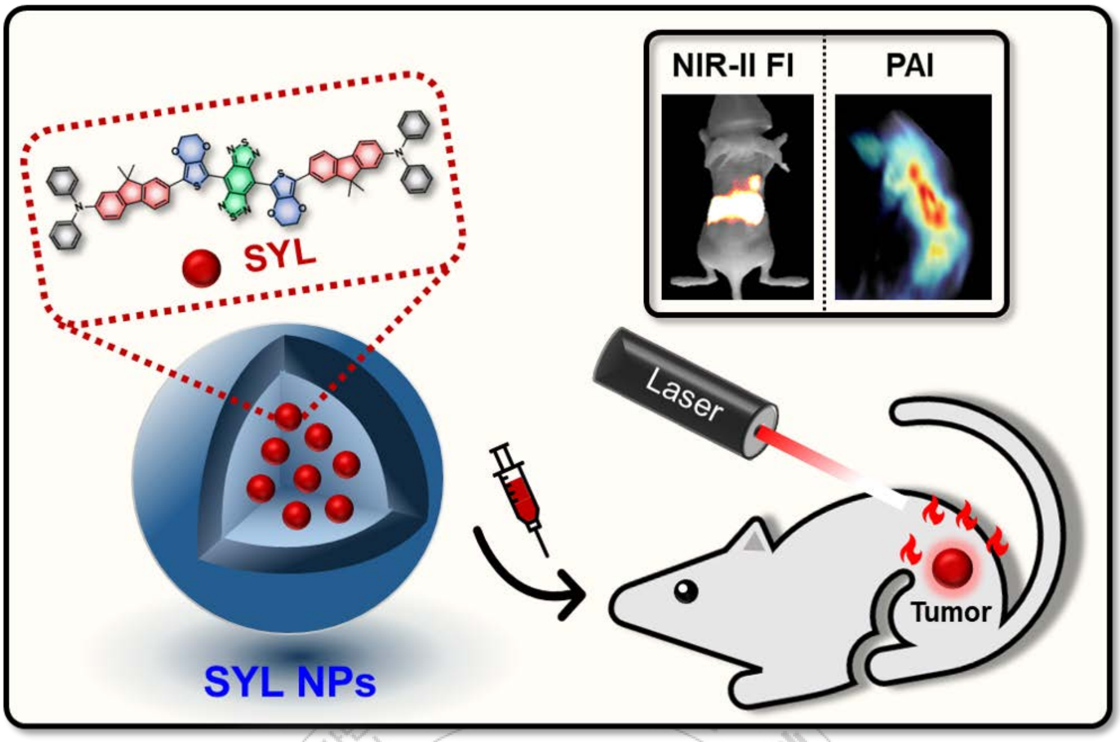
Exhibition Hall 1, FRI 11:00~12:30

Development of a theranostic platform with dual-modal NIR-ii/photoacoustic imaging and photothermal effect

Hyeong seok Kim, Subin Son, Ji Hyeon Kim, Jinwoo Shin, Jiseon Kim, Wonseok Choi, Jusung Ahn, Jongseung Kim*

Department of Chemistry, Korea University, Korea

A novel DD-A-DD scaffold molecular dye SYL was rationally designed and facilely synthesized with intrinsic multifunctional ability including dual-modal NIR-II fluorescence/PA imaging and photothermal therapeutic effect. SYL NPs based probe has the capability to passively target tumors in 4T1 subcutaneous mice model with not only relatively high fluorescence and photoacoustic signal outputs but also excellent S/B ratio. Additionally, the efficient tumor inhibition rate with minimal adverse side effects prolonged the life span of tumor-bearing mice in SYL NPs treated group under laser irradiation. It is highlighted that SYL NPs as a multifunctional platform could be an interesting candidate for cancer diagnosis (NIR-II) and therapy in future bio-applications


NIR-II FI
PAI
SYL
Laser
SYL NPs
Tumor

Poster Presentation : **ORGN.P-347**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Thermal phase behaviors of dicationic pyridinium salts

A Reum Lee, JongChan Shin, Minjae Lee[*]

Department of Chemistry, Kunsan National University, Korea

A series of *α,ω*-bis[*N,N'*-(4-alkylpyridinium)]alkane salts are synthesized and characterized. The synthetic route includes coupling reactions of 4-alkylpyridines with dibromoalkanes and anion-exchange reactions are following from the corresponding bis-pyridinium bromide salts. The synthesized bis-pyridinium salts contain either ethylene (C_2), propylene (C_3), or butylene (C_4) bridge between the pyridinium cations. The Tf_2N^- salts are thermally more stable than the PF_6^- salts with the same cation structure from thermogravimetric analysis. The C_3- and C_4-bridged bis-pyridinium salts are thermally more stable than C_2-bridged ones. The melting points of the salts decrease as the longer alkyl side chain length for the C_3 and C_4-bridged bis-pyridinium salts. However, the most C_2-bridged bis-pyridinium PF_6^- salts are thermally decomposed before their melting transitions. Interestingly, the most C_2-bridged bis-pyridinium PF_6^- salts show one or multiple solid-solid phase transitions, which is a typical a feature of organic plastic and liquid crystals. Most of the bis-pyridinium Tf_2N^- salts show only one melting transition except 1,4-bis[*N,N'*-(4-methylpyridinium)]butane Tf_2N^-, which shows one solid-solid phase transition.

Poster Presentation : **ORGN.P-348**

Organic Chemistry

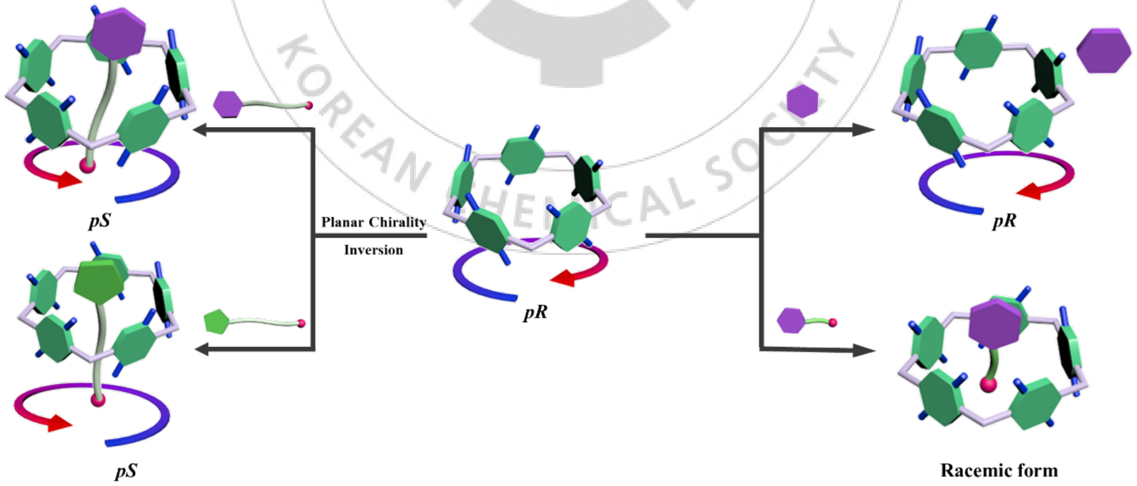
Exhibition Hall 1, FRI 11:00~12:30

Plannar Chirality Inversion of Alanine-Appended Pillar[5]arenes with Achiral Guest Molecules

Jaehyeon Park, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Planar chirality inversion of pillar[5]arenes bearing D- or L-alanine substituents on both rims wasinvestigated upon addition of guest molecules having pyridinium or imidazole moieties and long alkyl chains. The D- and L-alanine-substituted pillar[5]arenes exhibited *pS* and*pR* planar chirality, respectively. However, this planar chirality was inverted upon inclusion of certain achiral molecules, comprising pyridinium or imidazole moieties and long alkyl chains with terminal hydroxyl or methyl groups.



Poster Presentation : **ORGN.P-349**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Novel Activatable Prodrug for Overcoming Drug Resistance by Targeting Cancer Bioenergetics

Ji Hyeon Kim, Hyeong Seok Kim, Myung Sun Ji, Subin Son, Jinwoo Shin, Jiseon Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Nearly without exception, all known cancer chemotherapeutics elicit a resistance response over time. The resulting resistance is correlated with poor clinical outcomes. Here, we report an approach to overcoming resistance through reprogramming oncogene-directed alterations in mitochondrial metabolism before drug activation while simultaneously circumventing drug efflux pumps. Conjugate C1 increases cancer cell apoptosis and inhibits regrowth of drugresistant tumors, as inferred from efficacy studies carried out in human cancer cells and in Dox-resistant xenograft tumor models. It also displays minimal whole-animal toxicity. These benefits are ascribed to an ability to evade chemoresistance by switching cancer cell metabolism back to normal mitochondrial oxidative phosphorylation while helping target the active Dox to first the mitochondrion and then the nucleus.

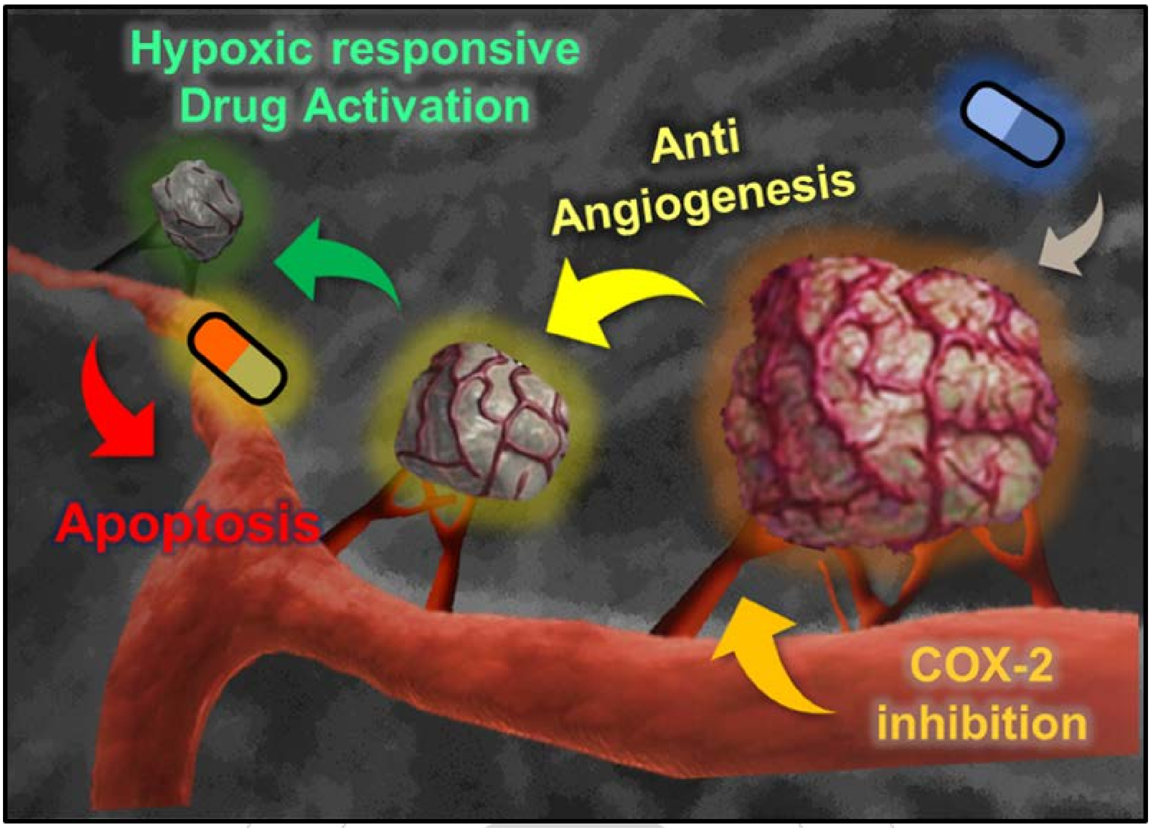
Poster Presentation : **ORGN.P-350**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Hypoxia-responsive Anti-angiogenic prodrug potentiates Cancer Therapeutic effect via COX-2 inhibition

Jusung An, Hyeong Seok Kim, Jinwoo Shin, Subin Son, Ji Hyeon Kim, Myung Sun Ji, Wonseok Choi, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Anti-angiogenesis, i.e., blocking the angiogenic pathway, has been considered as a significant strategy in current cancer therapy. However, the associated benefits have proven to be modest as tumor angiogenesis and regrowth persist, probably due to other ill-defined complex angiogenic mechanisms. Herein, we developed a cancer theranostic application consisted of indomethacin (IMC) incorporating system to mediate hypoxia responsive prodrug (TA) and diagnostic agent (DA). Cyclooxygenase 2 (COX-2) elevated expression in several cancer types is closely associated with severe tumor supporting vascularization factors. Utilizing COX-2 inhibition augmented the anti-angiogenetic induced hypoxia responsive prodrug activation well. Both in vitro and in vivo results proved that DA and TA exhibited specificity towards COX-2 positive (+ve) HeLa and A549 cancer cell lines and activation under hypoxic conditions. Compared with controls (R1, and anticancer drug SN-38), TA displayed prolonged tumor retention and enhanced therapeutic efficacy in xenograft mouse models at a reduced dosage. Our results considerably highlighted the importance of COX-2 blockade1,2 mediated anti-angiogenesis in complementing the hypoxia-responsive drug delivery systems (DDSs) and could to valuable for the brisk development of more progressive antitumor therapeutics.


Hypoxic responsive
Drug Activation
Anti
Angiogenesis
Apoptosis
COX-2
inhibition

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-351**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of N-1 Substituted 5-fluorouracil Derivatives and Testing for Inhibitory Effects of Cell Proliferation

Junghun Ha, Jong Hyun Cho*

Dong-A University, Korea

Recently, the development of many drugs can cure most diseases. However, side effects of the treatment process are still a problem to be solved. In this study, 5-FU(5-fluorouracil) derivatives were developed to improve the side effects of 5-FU. 5-FU is used as an anticancer agent for pancreatic and stomach cancers. However, side effects such as vomiting and diarrhea or myelosuppression exist. 5-FU is mainly used as a Thymidylate Synthase (TS) inhibitor. TS methylates dUMP to form dTMP and replicate DNA. 5-FU injections inhibit dTMP formation and kill cancer cells. Intermediate was synthesized by substituting the N-1 site of 5-FU. And the derivative was developed through esterification. The newly synthesized material was tested for the effect of inhibiting cell proliferation. A new active substance with reduced side effects was studied by synthesizing and developing a derivative based on 5-FU.

Poster Presentation : **ORGN.P-352**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Bioactivity evaluation of new Gallic acid derivatives with anticancer effects by Niche chemistry

Minhoe Gu, Ju Hyun Song*

Department of Chemistry, Dong-A University, Korea

Puer tea is very popular as diet food. There are various ingredients in the puer tea, including gallic acid. Gallic acid is a type of polyphenol, a natural antioxidant. It is also helpful for dieting. Lipase enzymes are enzymes that help absorb fat. Gallic acid inhibits the activity of lipase enzymes. Therefore, it prevents fat from accumulating in the body. Gallic acid also lowers levels of LDL cholesterol. Besides, the efficacy of gallic acid is varied. It acts as an anti-viral, anti-inflammatory and anti-allergy. Methyl gallate, one of the derivatives of gallic acid, has an anticancer effect. It has been proven that it effectively blocks the movement of T cells to inhibit cancer cell proliferation. For this reason, this study tries to develop a derivative of gallic acid. We hope to have a slightly better, slightly more diverse effect on the derivatives of various gallic acids.

Poster Presentation : **ORGN.P-353**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Acid-degradable Cationic Polyacrylates with 1,3,5-Hexahydrotriazine Core for Nucleic Acid Delivery

Jae Hun Jeong, Soo Kyung Cho[1,*]

Department of chemistry, Dong-A University, Korea

[1]*Division of Nano Convergence Technology, Pusan National University, Korea*

Dendrimer is used as a useful substance in the drug delivery system and has many advantages such as clear structure, various functionalities, and uniformity of molecules. However, due to the large molecular weight and large surface area, it can also cause toxic problems. Therefore, we propose a dendrimer that can be broken down into biologically harmless molecules after successful delivery of the drug. In this study, 1,3,5-hexahydrotrizine core is synthesized with amino acid (glycine,serine,cystein,etc).Triazacyclohexane core expects to increase flexibility to facilitate interaction with genes and, when degraded, break down into amino acids and alcohol and acetone and small molecules to reduce side effects such as toxicity to cells. And try to react a synthesized hexahydrotriazine derivative with salient carboxylic acids or alcohols to create a new drug that has no side effects and is less human-toxic and highly physiologically active.

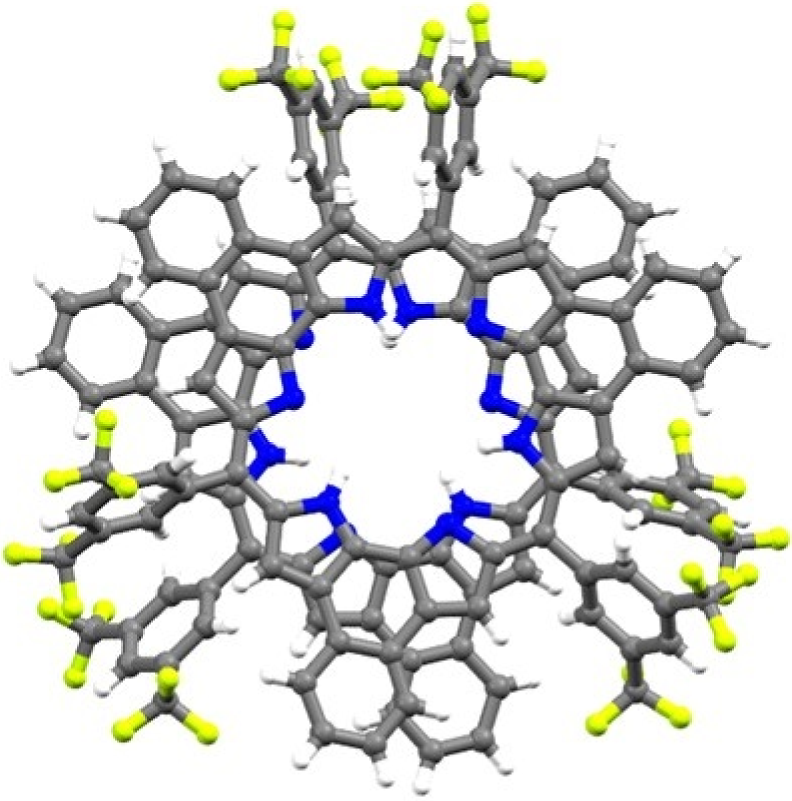
Poster Presentation : **ORGN.P-354**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Co-facially Stacked, Antiaromatic Hexaphyrin(1.0.1.0.1.0) Dimer

Chang Hee Lee*, Ranjan Dutta

Department of Chemistry, Kangwon National University, Korea

Parallel alignment of π-conjugated molecules offers electronic communication through orbital overlap. Qualitative frontier orbital analysis suggests that a parallel “face-to-face” orientation of two aromatic rings should result in their repulsive interaction. Conversely, the analogous interaction of two stacked antiaromatic rings should lead to stabilization. Recently, we have reported offset stacking of 24-π antiaromatic hexaphyrin bearing pentafluorophenyl groups as meso-components. We envisioned that installation of suitable meso-substituents could enable this particular system to undergo spatial reorganization to form a “face-to-face” stacked hexaphyrin oligomer(s). A judicious screening of aromatic aldehydes based on their reactivity and steric elements, we found 3,5-bis(trifluoromethyl)bezaldehyde displayed our desired objectives. For instance, co-facial stacking of this particular hexaphyrin with short π-π distance (3.39 Å) is noted in solid state. Gratifyingly, this discrete dimeric species persists in solution as an equilibrium mixture of monomer and dimer. Notably, both monomer and dimer could be distinguished by their distinct spectral features. Synthesis, characterizations and qualitative evaluation of its antiaromatic features will be presented.



Poster Presentation : **ORGN.P-355**

Organic Chemistry

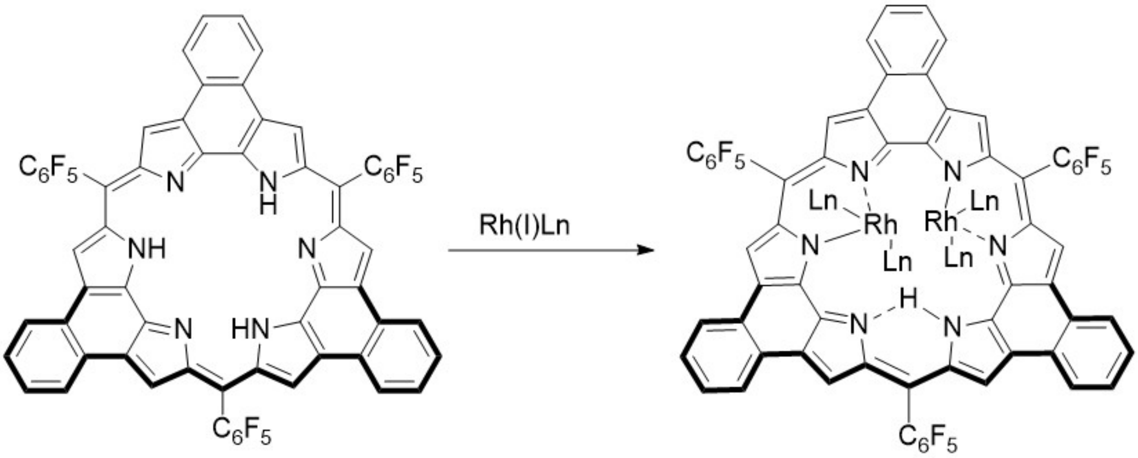
Exhibition Hall 1, FRI 11:00~12:30

Bimetalic Rhodium (I) Complex of Anti-aromatic, pi-Extended Planar Hexaphyrin[1.0.1.0.1.0]

Chang Hee Lee*, Srinivas Samala[1], Ranjan Dutta, Qing He[2], Vince Lynch[3], Jonathan Sessler[3]

Department of Chemistry, Kangwon National University, Korea
[1]*Chemistry, Kangwon National University, Korea*
[2]*Chemistry, Hunan University, Korea*
[3]*Chemistry, University of Texas, Austin, Korea*

Porphyrins are well known aromatic macrocycles with 18pi electronic system, usually forms stable metal complexes with various transition metals with maintaining original aromatic character. In recent years metaloporphyrins are became attracted considerable attention due to their useful chemical and optoelectronic properties. Now we have been interested in the synthesis of metal complexes of pi-expanded porphyrins, particularly rosarin, which is stable anti-aromatic (24-pi) compound with near planar geometry. Surprisingly, to the best of our knowledge, till now there is no report for the anti-aromatic rhodium(I) complexes. Here, we report the first synthesis of bimetallic Rh(I)-rosarin complex along with full characterization by spectroscopic means including single crystal X-ray analysis. The study revealed that the complex retains anti-aromatic characteristics and accommodate two rhodium (I) metals in the core. Each rhodium adopts square planar geometry. The resonance of the remaining one pyrrole N-H appears at ~33 ppm in 1H NMR spectrum and it is strongly resistant to exchange with deuterium. The synthesized rhodium (I) complex is stable in strongly acidic solution. Details for the structural and spectroscopic properties will be presented.


C6F5
N
NH
C6F5
NH
N
N
HN
C6F5
Rh(I)Ln
C6F5
N
N
Ln
Rh
Ln
Rh
Ln
Ln
N
N
N
H
N
C6F5
C6F5

Poster Presentation : **ORGN.P-356**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Bidentate Imidazo[1,5-*a*]pyridine *N*]-Heterocyclic Carbene Nickel(II) Complexes for Acrylate Synthesis from Ethylene and CO_2.

Jiyun Kim, Ji Yeon Ryu[1], Junseong Lee[1], Sukwon Hong*

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

A series of novel bidentate imidazo[1,5-*a*]]pyridine-3-ylidene (ImPy) ligands and their nickel(II) complexes were synthesized for catalytic synthesis of acrylate from ethylene and CO_2, which is one of the future application in CO_2 capture and utilization (CCU). The bidentate ImPy based nickel(II) complexes ImPy-Ni(II)Br_2 were generated by transmetalation via silver precursors. Their molecular structures with structurally strong chelating effect were confirmed based on the X-ray crystal analysis. The bidentate ImPy-nickel(II) complexes exhibit catalytic activities in acrylate synthesis from ethylene and CO_2 (turnover number up to ***). Considering bisphosphine ligands have been typically used in this transformation, the current results with bidentate ImPy-Ni(II) catalysts could deserve attention.

Poster Presentation : **ORGN.P-357**

Organic Chemistry

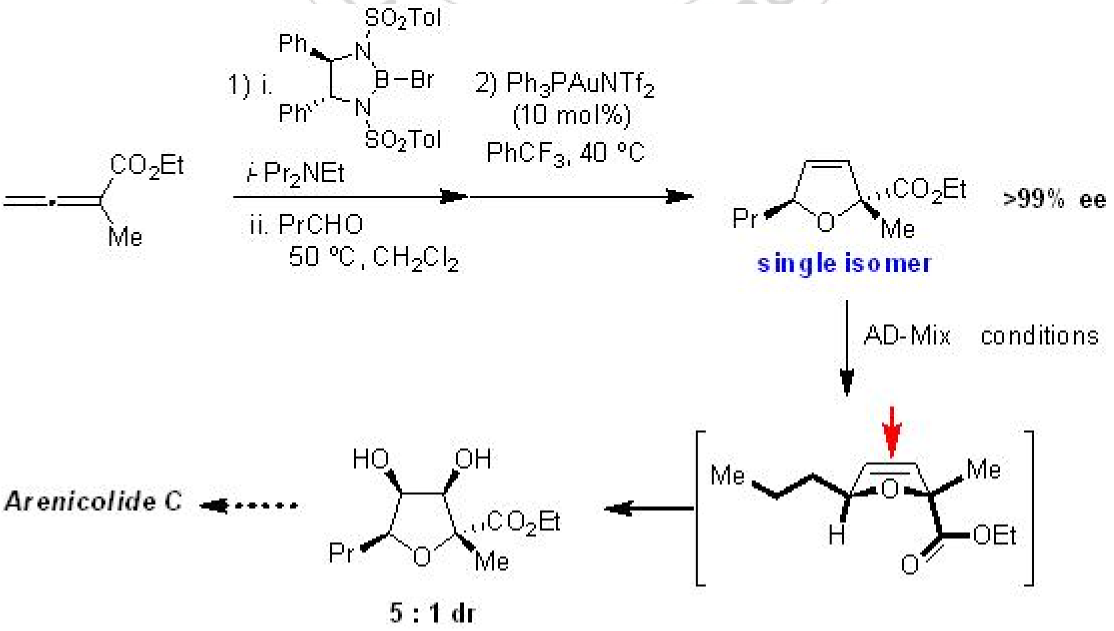
Exhibition Hall 1, FRI 11:00~12:30

Facile Synthesis of Highly Functionalized tetrahydrofuran through Allenoate Gamma-addition/Gold Catalysis followed by ADD: Construction of Cytotoxic Arenicolide C Unit

Euijin Park, Gyungah Pak, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

During the past few decades, substantial progress has been made for a variety of diastereoselective methods mediated by chiral reagents and catalysts. Recently, we disclosed discoveries of an unprecedented gamma-addition of 2-alkyl allenoates with a chiral bromoborane in the presence of iPr2NEt, followed by addition of aldehydes to establish central and axial chirality. We present herein a new method for the stereospecific synthesis of dihydrofuran derivatives via gold cyclization as described below. We also describe synthetic application to anticancer reagent arenicolide C unit including reaction conditions, scope and limitation of the reaction.



Poster Presentation : **ORGN.P-358**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Copper-catalyzed one-pot synthesis of functionalized 2-quinolones.

Ah Reum Kim, Jongseung Kim, Hee Nam Lim[1,*]

Department of Chemistry, Korea University, Korea
[1]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

2-Quinolones are significant structures in medicinal and material chemistry. They are also found in a number of natural products and biomaterials. Herein, we developed a copper-catalysis for synthesis of 3,4-difunctionalized 2-quinolones; this is enabled by the one-pot cascade reaction via S_N2, C-N bond coupling, and Knoevenagel reaction. A diverse set of the functionalized 2-quinolone library was prepared by this protocol. This method highlights easy reaction set-up in open-air condition, thus being more user-friendly.

Poster Presentation : **ORGN.P-359**

Organic Chemistry

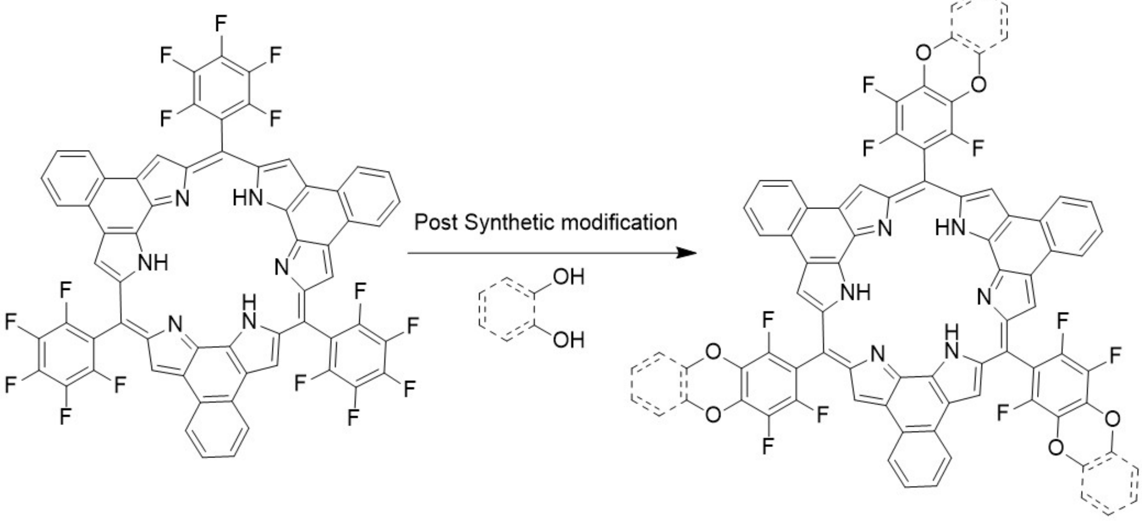
Exhibition Hall 1, FRI 11:00~12:30

Post synthetic modification of antiaromatic, β,β’-phenylene fused hexaphyrin [1.0.1.0.1.0]

Chang Hee Lee*, Brijesh Chandra[1]

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

β,β’-phenylene fused hexaphyrins (1,0,1,0,1,0) have served as one of the best model to explore the aromaticity issue and can exist in various electron state during redox reactions. We developed β,β’-phenylene bridged, ring annulated hexaphyrin (1.0.1.0.1.0) trivially called as ‘Rosarin’, is planer 24π-electron antiaromatic system that displayed protonation coupled electron transfer (PCET) phenomenon. We have taken a step further to develop new rosarins with enhanced redox properties, by post synthetic modification. Our nucleophilic aromatic substitution approach at meso-pentafluorophenyl group of rosarin has led to develop new modified rosarins. The synthesis resulted in the formation of tri-substituted rosarin. Full characterization, their optical properties and redox behavior will be presented in the poster.



Poster Presentation : **ORGN.P-360**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Total Synthesis of Taxamairin B via an Intramolecular Heck Reaction

Chang Ho Oh*, Le Thuy Quynh[1], Uiseong Chai[2]

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

A green strategy towards the total synthesis of Taxamairin B has been described. Intramolecular Heck works efficiently to furnish 6-7-6 fused icetexane scaffold under hydrative condition, which on restructuring affords the key intermediate β,γ-enedione. The later on selective oxidation transforms into Taxamairin B.This method is flexible to construct 6-7-6 scaffold of icetexane diterpenoids and other natural products having this molecular framework.

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Poster Presentation : **ORGN.P-361**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Theranostic Agent based on Glycyrrhetinic Acid Structure for Hepatocellular Carcinoma

Myung Sun Ji, Subin Son, Jinwoo Shin, Jusung An, Ji Hyeon Kim, Wonseok Choi, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Conventional chemotherapies have severe side effects because of non-specificity and systemic toxicity of anti-cancer drug to normal tissues and organs. Targeted delivery of anticancer drugs to cancer could be beneficial to overcome the side effect and cancer associated mortality. Using active targeting ligand which can bind to specific receptors overexpressed on cancer cells is one of the acclaimed strategies. Herein, we will present our findings regarding exploring the glycyrrhetinic acid (GA) as an active targeting ligand for hepatocellular carcinoma (HCC) on a small molecule-based approach for imaging and therapeutics. Our preliminary in vitro results suggested that GA-modification can enhance the cellular uptake of conjugates, specifically by liver cancer cell lines (HepG2 and Chang liver cells) via GA selective endocytic pathway. Furthermore, in vivo studies with HepG2-inoculated xenograft models successfully demonstrated that prodrug displayed efficient tumor targeting with enhanced cytotoxicity which may be attributed to prodrug activation by enzyme-mediated ester hydrolysis followed by self-immolative release of active drug, epirubicin (EPI).

Poster Presentation : **ORGN.P-362**

Organic Chemistry

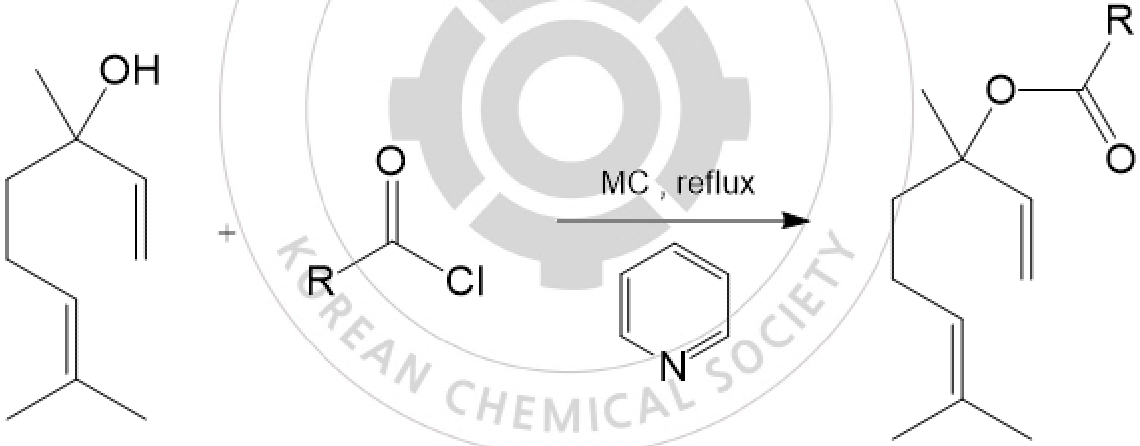
Exhibition Hall 1, FRI 11:00~12:30

Application and Synthesis of Linalool Derivatives as Aroma Chemicals

JiEun Lee, **Chuljin Ahn***

Department of Biology and Chemistry, Changwon National University, Korea

The linalool derivatives have been used as aroma chemicals. The known and new linalool derivatives were prepared conveniently in our lab, and were investigated their fragrance.



R : iso-butyl, Methyl, Naphthoyl, Phenyl, etc.

Poster Presentation : **ORGN.P-363**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

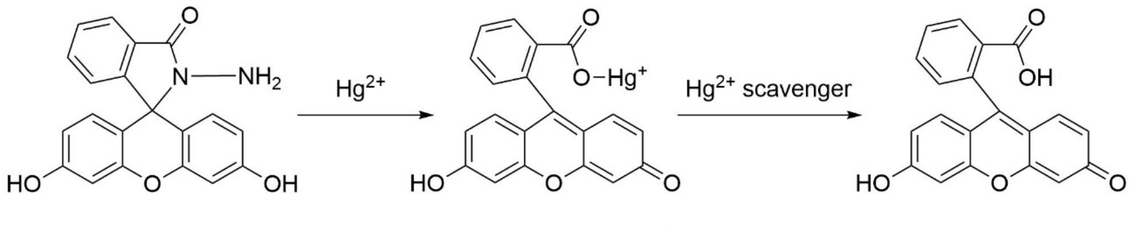
Visible readout by Interfacial photo-polymerization comparing with Absorption and Fluorescence using Hg(II)-fluorescein hydrazide complex

Hyungwook Kim, Young Jae Jung[1], JungKyu Lee*

Department of Chemistry, Kyungpook National University, Korea

[1]*Kyungpook National University, Korea*

The use of polymers for detection of a molecular recognition events was reviewed by K. Kaastrupa, & H. D. Sikes1) and Scrimin, P., & Prins, L. J.2) and is attractive due to simplicity, turnability and performance as well as being detected with naked eye. Interfacial photo-polymerization system was reported that it forms ticker hydrogel in a shorter reaction time than other polymerization-based amplification(PBA) with similar sensitivity.3) The cross-linked polymer which is an interfacial photo-polymerization based on a visible-light induced photoredox catalysis was produced by reaction of poly(ethylene glycol) diacrylate (PEGDA), 5-vinyl-2-pyrrolidone(VP), Triethanolamine(TEOA) and Fluorescent dye that does intersystem-crossing. We attempt to detect Hg^{2+} in aqueous solution and determine lower limit, to confirm the extensibility of this system in chemical detection. This method was compared, using Absorption and Fluorescence spectroscopy. Fluorescein Hydrazide was used to detect Hg^{2+} concentration on aqueous solution, since it turns on the absorption and fluorescence after forming Fluorescein hydrazide-Hg^{2+} complex. Furthermore, the signal was amplified by using a scavenger to drop mercury from the complex. In the current system, Detection limit of PBA and absorption were 1uM and fluorescence was 30nM (6μg/L) which was recommended for drinking water quality in the WHO. In addition, the reaction rate constants of Fluorescein Hydrazide-Hg^{2+} complex were calculated with temperature and time. After, we will attempt to see the hydrogel with a concentration under 30nM, using another visible light induced photo-reduction catalyst or a photo-initiator in which mercury is catalyzed.Referense1) K. Kaastrup and H. D. Sikes , Chem. Soc. Rev., 2016,45, 532-5452) P. Scrimin and L. J. Prins , Chem. Soc. Rev., 2011, 40 , 4488-45053) K. Kaastrup and H. D. Sikes , Lab Chip, 2012, 12 , 4055 -4058



A) Fluorescein Hydrazide (FH) B) FH-Hg(II) complex[1)] C) Fluorescein

Poster Presentation : **ORGN.P-364**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

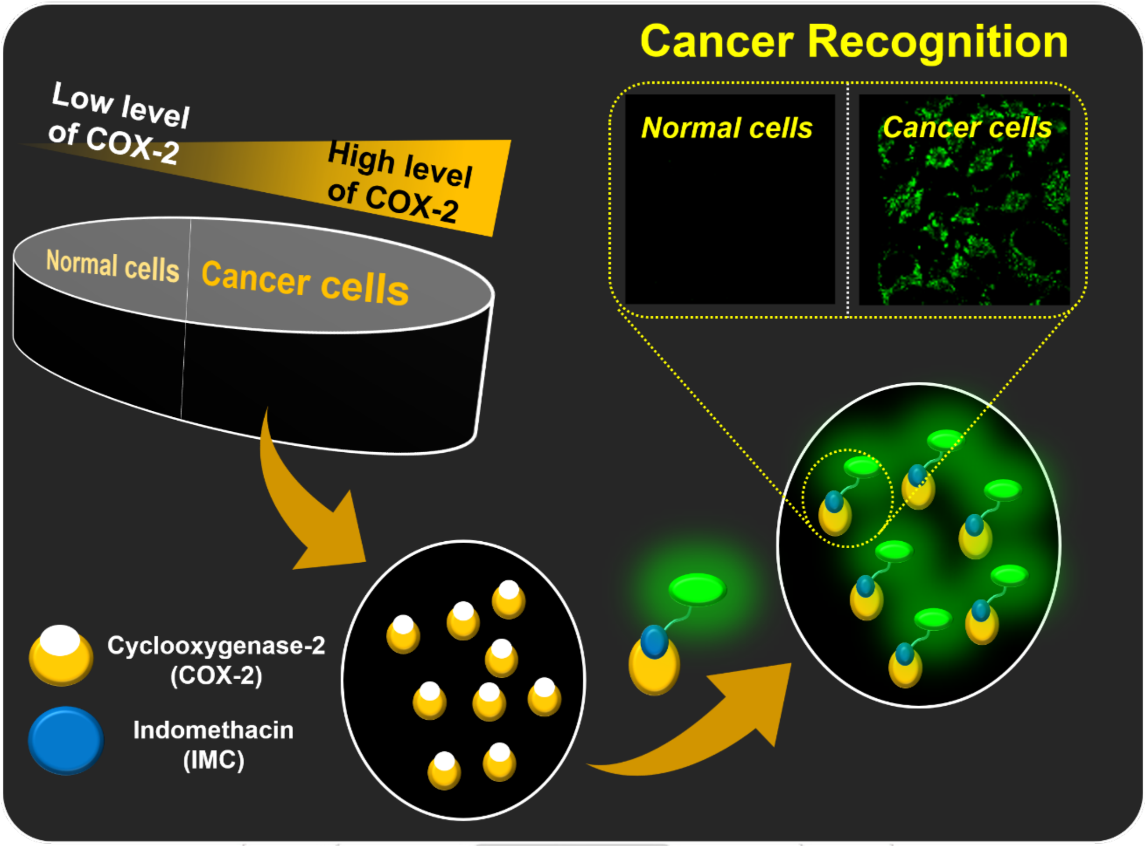
An Indomethacin guided fluorescent probe for targeting cyclooxygenase 2 (COX-2) can discriminate cancer cells over normal cells

Zehra Zunbul, Hyeong Seok Kim[1], Jongseung Kim[1,*]

Chemistry, Korea University, Turkey

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

The COX-2 targeting indomethacin-conjugated fluorescent probe, IQ-1, was designed and synthesized for selective fluorescence imaging of cancer cells over normal cells. IQ-1 showed stronger fluorescence imaging of COX-2 overexperessing cancer cells (OVCAR3, HepG2 and Hela cells) than of normal cell lines (RAW 246.7 and fibroblast cells). For clarifying COX-2 targeting ability of IQ-1, LPS as an oxidative stress agent, treated inflamed cell lines inducing high COX-2 levels also revealed an enhanced fluorescence. As inhibitory studies, it was tested that cancer cells was co-treated with COX-2 inhibitors such as indomethacin and aceclofenac, resulting in a markedly reduced fluorescence intensity. Therefore, IQ-1 can be used as a selective bioimaging agent for cancer cells over normal cells, and could be developed for efficient diagnosis and therapeutic monitoring in precision medicine.


Cancer Recognition
Low level of COX-2
High level of COX-2
Normal cells
Cancer cells
Normal cells
Cancer cells
Cyclooxygenase-2 (COX-2)
Indomethacin (IMC)

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Poster Presentation : **ORGN.P-365**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Asymmetric Total Synthesis of (-)-Bulgecinine via Regioselective and Diastereoselective Amination Using Chlorosulfonyl Isocyanate

Yong Sun Cho, Ji Eun Kang, Young Hoon Jung*

School of Pharmacy, Sungkyunkwan University, Korea

Bulgecinine, one of nonproteinogenic amino acid component, is a aglycon of potent β-lactam synergist bulgecin which was generated during the fermentation of two Gram-negative bacteria, P.mesoacidophila and Pseudomonas acidophila. The combination of β-lactam antibiotics and bulgecin formulates bulge and that increases organism sensitivity to inhibition, therefore the β-lactam concentration decreases and consequently sets harsh condition to survival of bacteria.The class of bulgecinine structure is polyhydroxylated piperidines, azasugars. Azasugar moiety is one of most prevalent structure of natural products. Mimicking the natural sugars that have similar moiety, they can bind to the specific active sites of glycosidases. Thereby a number of azasugar compounds prevent numerous diseases from affecting patients, including diabetes, AIDS, cancer and viral infections. Using chlorosulfonyl isocynate(CSI) reagent, we have developed a variety of methods to institute amino group regioselectively and diastereoselectively. As a result, we can prepare lots of asymmetric total synthesis of biologically active natural compounds. We herein describe an asymmetric total synthesis of (-)-bulgecinine starting from readily available α-methyl-D-mannosideEspecially high regioselectivity and diastereoselectivity(anti:syn = 14:1) were observed in represented amination reaction to achieve carbamate compound from corresponding polybenzyl ether. The pathway of SNi type reaction with neighboring effect is introduced to elucidate the proposed mechanism.

Poster Presentation : **ORGN.P-366**

Organic Chemistry

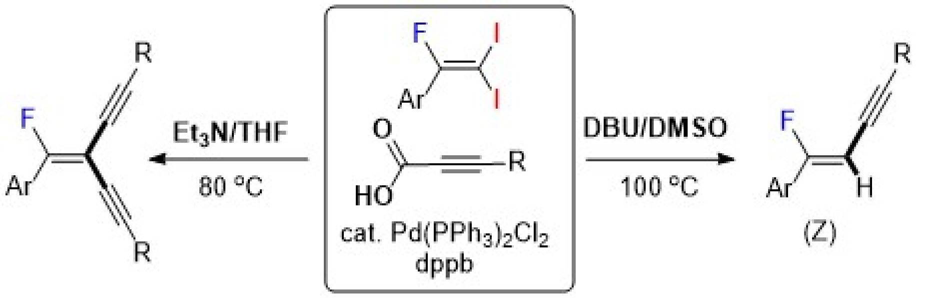
Exhibition Hall 1, FRI 11:00~12:30

Selective Mono- and Di-alkynylation of 2-fluoro-1,1-diiodovinylarenes using Pd-catalyzed Decarboxylative Coupling Reactions

Joseph Devaneyan, **Sunwoo Lee***

Department of Chemistry, Chonnam National University, Korea

Palladium-catalyzed decarboxylative coupling reactions using alkynoic acids and 2-fluoro-1,1-diiodovinylarenes provide mono- and dialkynyl fluoroalkenes with high selectivity. When the reaction was conducted using DBU/DMSO, the hydrodeiodinated monoalkynyl fluoroalkene product was formed, whereas performing the reaction using Triethylamine/THF gave the dialkynyl fluoroalkene product. Both reaction conditions gave high yields of the desired enynes and endiynes products bearing fluorine atoms.



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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

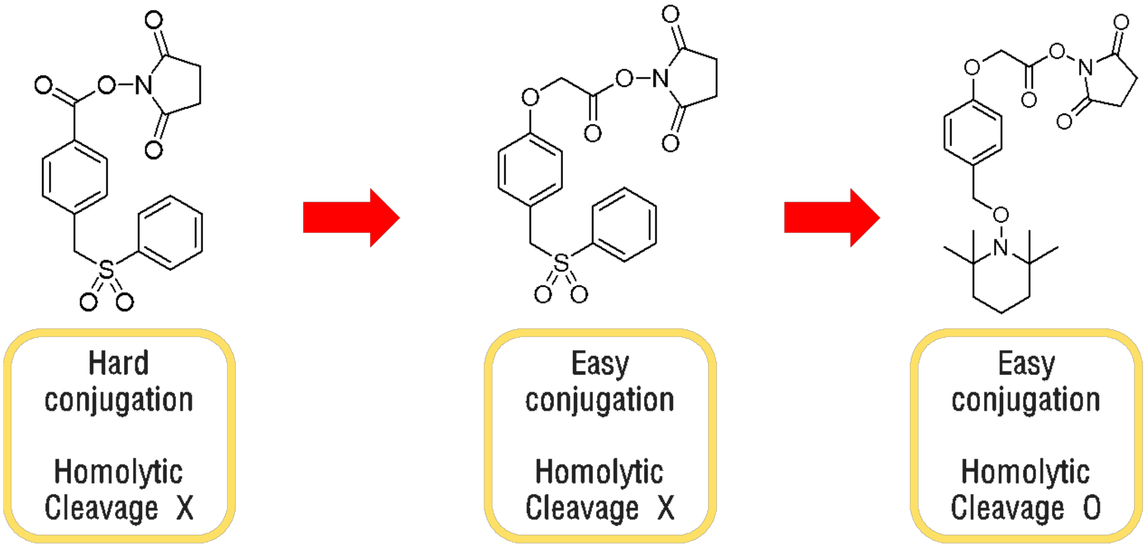
Poster Presentation : **ORGN.P-367**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Design and synthesis of homolytically photocleavable compound for Free Radical-Initiated Peptide Sequencing Mass spectrometry (FRIPS MS)

Jiho Park

chemistry, Sogang University, Korea

Free radical-initiated peptide sequencing mass spectrometry(FRIPS-MS) is one of the powerful tools for peptide sequencing analysis. These technique requires a specific functional group that can be cleaved under the high-energy gas molecule collision conditions to pruduce a radical species. When a biomolecule such as angiotensin II tagged with a FRIPS-MS mass tag run through tandem mass spectroscopy, two free radicals are generated at specific functional group because of the homolytic cleavage and the sequential fragmentation through a radical mechanism. The free radicals attack the peptide bond in biomolecule then the bond is cleaved by-ax or -cz form. In our previous experiments, we tested benzenesulfonyl group which can be used as another cleavage group replacing TEMPO free radical (2,2,6,6-tetramethyl-1-piperidinyloxy free radical). In addition we have changed the balance group to improve the homolytic cleavage. In conclusion, benzenesulfonyl group cannot work for homolytic cleavage. However, we recognized that the bioconjugation efficiency with biomolecules can be improved by functional group modification at the balance group. We assumed that the homolytic cleavage could be activated if the cleavage bond becomes more electron deficient. Although it did not work ideally, we observed improving conjugation by introduced EDG at para-position of balance group. With this observation, FRIPS-MS tag was re-designed and synthesized employing TEMPO. Homolytic cleavage is generated in MS/MS and also the desired specific mass fragmentation (e.g. -ax or -cz from) was observed with this new tag.


Hard conjugation
Homolytic Cleavage X
Easy conjugation
Homolytic Cleavage X
Easy conjugation
Homolytic Cleavage O

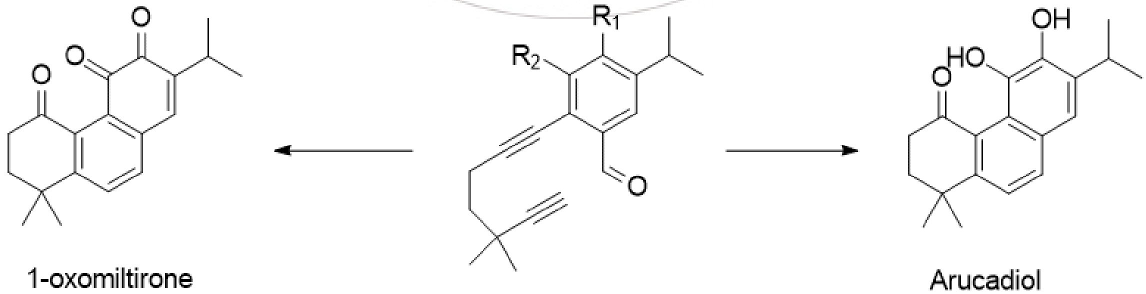
Poster Presentation : **ORGN.P-368**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Synthesis of abietanes via Gold and Copper-Catalyzed Cyclization as Key Steps

Chaehyeon Seong, Juyeon Kang, Uiseong Chai, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

Salvia, a herb belonging to the family Lamiaceae is found around 500 species worldwide. Diterpenoids content and taxonomic and molecular phylogenetic analysis are reported in this kind of chemical studies of diverse salvia species, usually known as salage, which have proved that diverse and definite secondary metabolites are diterpenoids. Attracted by the structural characteristics as well as the biological activity of Abietanes compounds, several groups have been interested in the synthesis of adietanes compounds. Transition-metal-catalyzed cycloisomerization of polyunsaturated systems is an atomic-economical and environmentally friendly synthetic method that allows efficient access to building blocks useful in various structural motifs and synthetic chemistries of many natural products. In this paper, we will describe a short synthesis of arucadiol and its analogs from products obtained from gold and copper-catalyzed cycloisomerization of ynals with pendant alkyne.



1-oxomiltirone
R_1 = H., R_2 = OMe

Arucadiol
R_1 , R_2 = OMe

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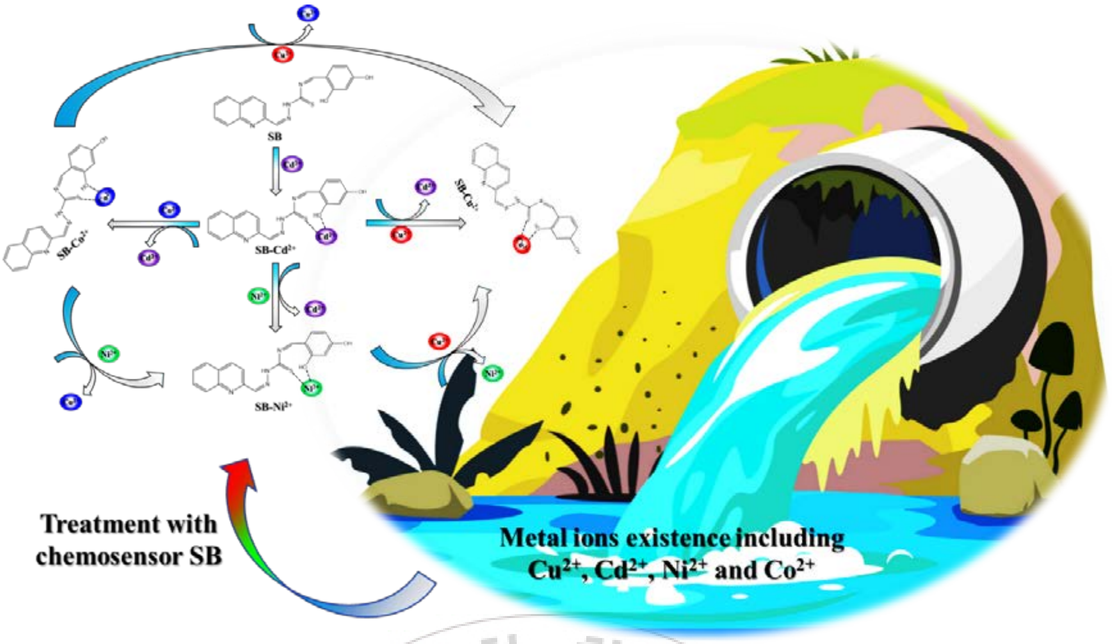
Poster Presentation : **ORGN.P-369**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A multi-responsive Schiff base as dual mode chemosensor for colorimetric and fluorometric detection of heavy metal ions at nano-molar levels

Prasad Gajanan Mahajan, Nilam Chandrakant Dige[1], Balasaheb Daniyal Vanjare, Ki Hwan Lee[*]

Department of Chemistry, Kongju National University, Korea
[1]*Department of Biological Sciences, Kongju National University, Korea*

A Schiff base centered chemosensor SB has been synthesized and further utilized for the selective and sensitive detection of four metal ions through dual channels, those were based on absorption and fluorescence properties. The distinguishing recognition of Ni2+, Cu2+, Co2+ and Cd2+ in an aqueous solution was performed by observing naked eye rapid color change, absorption and fluorescence spectrum of chemosensor SB in the absence and in the presence of specific metal ion at respective concentration. The detection method based on absorption studies offers detection limit of 0.224 nM, 0.656 nM, 1.047 nM and 1.043 nM for Cu2+, Ni2+, Co2+ and Cd2+, respectively. While, limit of detection based on fluorescence method for Cu2+, Ni2+, Co2+ and Cd2+ was found to be 0.184 nM, 0.637 nM, 1.053 nM and 1.070 nM, respectively. The mechanism for change in absorption and fluorescence properties of SB involves formation of ground state non-fluorescent complex through static quenching process. The theoretical calculations based on TD-DFT studies are in support of experimental interpretations.


SB
SB-Cd²⁺
SB-Co²⁺
SB-Cu²⁺
SB-Ni²⁺
Treatment with chemosensor SB
Metal ions existence including Cu²⁺, Cd²⁺, Ni²⁺ and Co²⁺

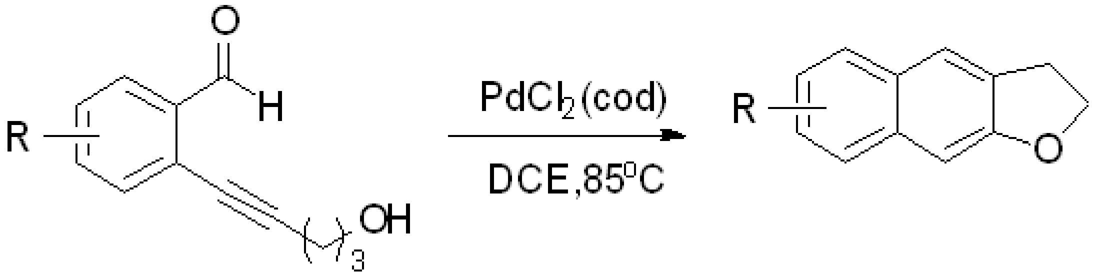
Poster Presentation : **ORGN.P-370**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis via Palladium-Catalyzed Cyclization of 2,3-Dihydronaphtho[2,3-b]furan

SeungLyeol Lee, **Le Thuy Quynh**[1], **Chang Ho Oh**[*]

Department of Chemistry, Hanyang University, Korea
[1]*Chemistry department, Hanyang University, Korea*

2-(5-hydroxypent-1-yn-1-yl)benzaldehyde has been synthesized by the sonogashira reaction of 2-bromobenzaldehydes with 5-pentyn-1-ols. The synthesis of oxycyclic naphthalenes have been reported already by utilizing ortho-formylacetylenols (n = 3) via AuCl3-or AgTFA- annulations. We have found the synthesis of 2,3-dihydronaphtho[2,3-b]furan with the aldehyde precursors when PdCl2(cod) was employed as the catalyst. As well as, in this case the conversion of 2,3-dihydronaphtho[2,3-b]furans was close to 100%. We have attempted to applied via palladium-catalyzed cyclization to 2,3-dihydronaphtho[2,3-b]furans which were substituted variously.



Poster Presentation : **ORGN.P-371**

Organic Chemistry

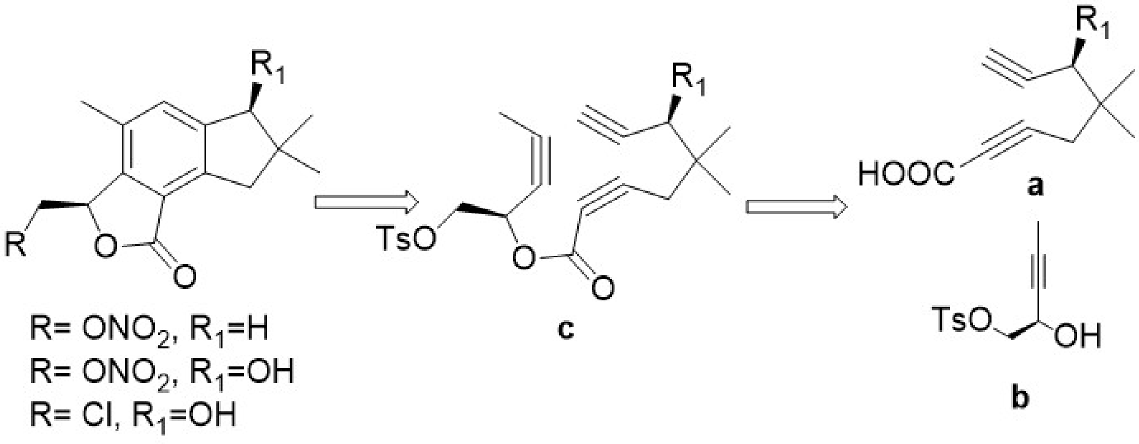
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of marine illudalane sesquiterpenoid Alcyopterosin series via [2+2+2] triyne cyclization.

Juyeon Kang, Jegeun Jo, Chang Ho Oh*

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.



Scheme 1. Retrosynthesis of Alcyopterosin E, L, M

Poster Presentation : **ORGN.P-372**

Organic Chemistry

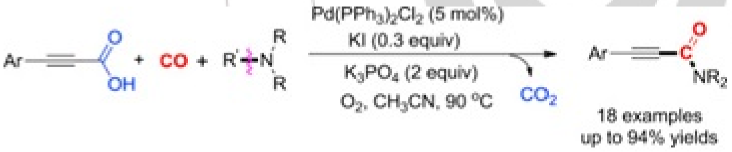
Exhibition Hall 1, FRI 11:00~12:30

Palladium-catalyzed decarboxylative aminocarbonylation with alkynoic acid and tertiary amine for the synthesis of alkynyl amide

Muhammad Aliyu Idris, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

We developed a method for the synthesis of alkynyl amides via the carbonylation of alkynoic acids and C-N activation of tertiary amines. The reaction of alkynoic acid and tertiary amine with carbon monoxide using a palladium catalyst in the presence of oxygen, Potassium iodide, and Tripotassium phosphate, gave the desired alkynyl amides in good yields



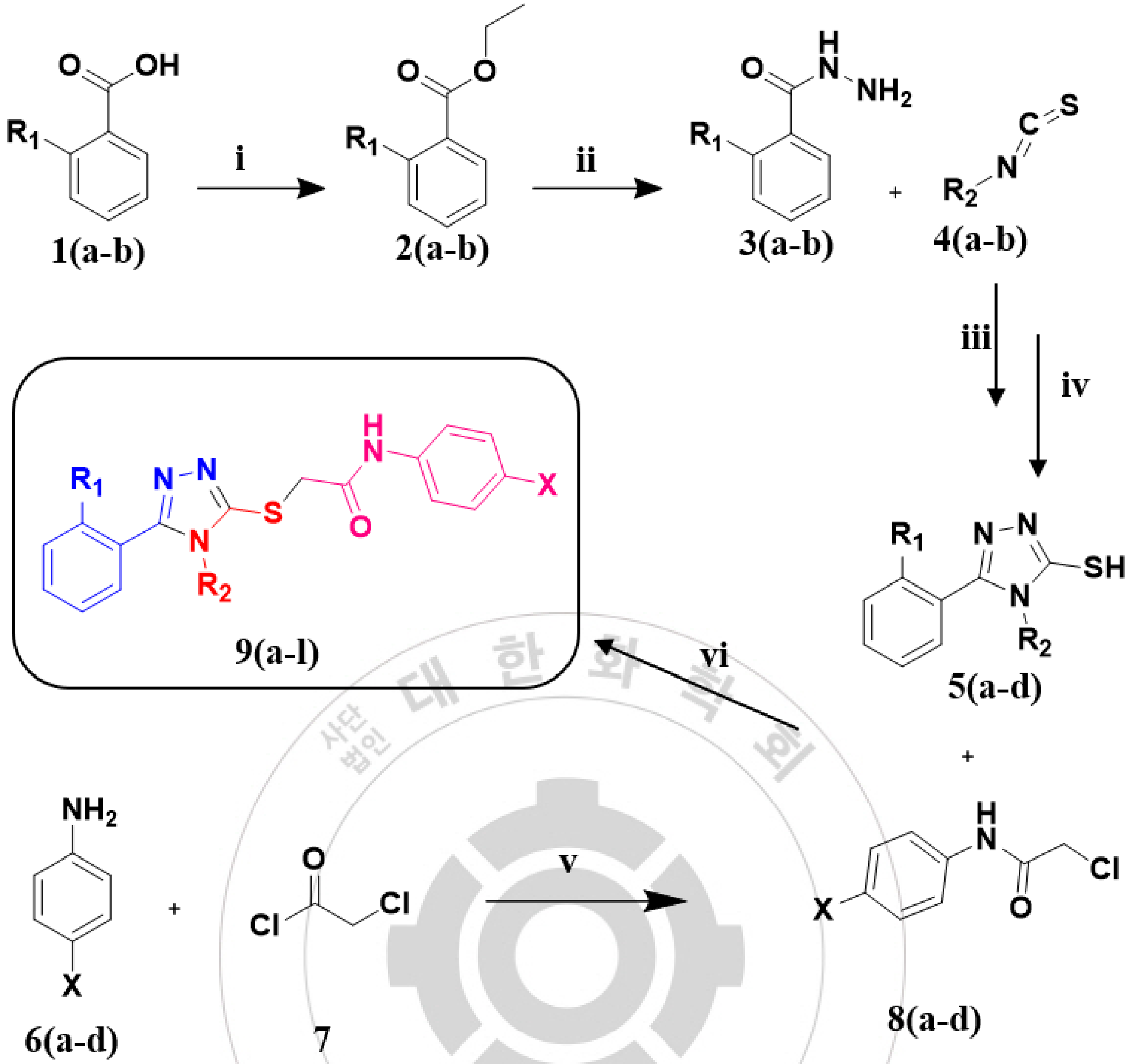
Poster Presentation : **ORGN.P-373**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Structural Activity Relationship of Mushroom Tyrosinase Inhibiting Novel 1, 2,4-Triazole Based Derivatives: Kinetic Mechanism, Molecular Docking and Dynamic Simulation Insights

Balasaheb Daniyal Vanjare, Ki Hwan Lee*, Prasad Gajanan Mahajan, Nilam Chandrakant Dige[1]

Department of Chemistry, Kongju National University, Korea
[1]*Department of Biological Sciences, College of Natural Science (Building No. 11), Korea*

A series of 12 new 1, 2, 4-triazole based derivatives have been designed and synthesized. The target compounds 1, 2, 4-triazol-3-ylthio)-N-(phenyl) acetamide derivatives (9a-9l) were synthesized by the reaction of 4 and 5 substituted 1, 2, 4-triazole-3-thiol derivatives (5a-5d) with 2-chloro-N-un/substituted phenyl acetamide derivatives (8a-8d) under basic condition. The structural confirmation has been assessed by using FT-IR, LC-MS, 1H NMR and 13C NMR method. All the synthesized compounds (9a-9l) were screened for biological activity (Mushroom Tyrosinase inhibition potential) and all derivatives demonstrates a great results. Nevertheless, compound 9k (0.0048±0.0016 μM) exhibit 3500 times more active compared with standard drug Kojic acid (16.8320±1.1600 μM) against mushroom tyrosinase inhibitor. The molecular docking study delivers the idea about the interaction of the ligand with an enzyme. Additionally, the dynamic simulation was accomplished for compound 9k to govern the plausible binding model.


1(a-b)
i
2(a-b)
ii
3(a-b)
+
4(a-b)
iii
iv
5(a-d)
+
9(a-l)
vi
6(a-d)
+
7
v
8(a-d)

Poster Presentation : **ORGN.P-374**

Organic Chemistry

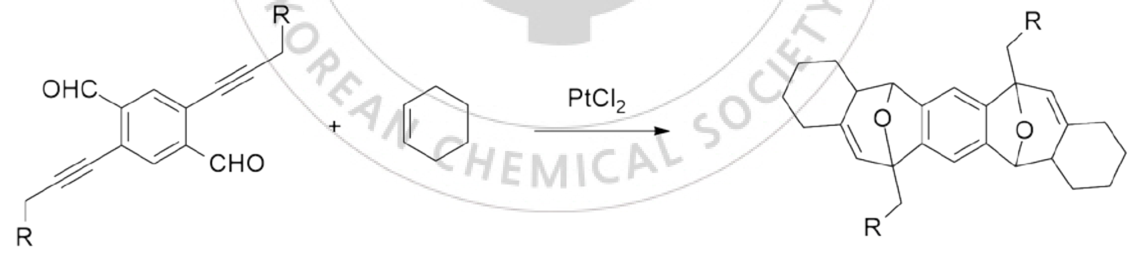
Exhibition Hall 1, FRI 11:00~12:30

The bisannulation applying platinum-catalyzed cyclization of o-alkynyl benzaldehyde to synthesis polycyclic compound containing 7-membered rings.

Uiseong Chai, Chang Ho Oh[*]

Department of Chemistry, Hanyang University, Korea

We tried to apply the platinum-catalyzed cyclization through bezonpyrylium intermediate and [3+2] cycloaddition of an alkene, to 2,5-dialkynylterephthaldehyde. We check the possibility of bisannulation depending on the substrates and kinds of alkenes, and discuss why the bisannulation has different result when compared to monoannulation. The outcome of bisannulation shows unique structure, two 7-memebered rings are sandwiching a central benzene.



R= OBn, OTBS, CH2CH2CH3

Poster Presentation : **ORGN.P-375**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Design and Synthesis of a New fluorescent TEMPO-FRIPS Reagent for Glycan Analysis

Gunwoo Kim

chemistry, Sogang University, Korea

Glycans are very important because they are involved in various biological processes. There are many ways to analyze glycans, but mass spectrometry has been extensively used as a powerful tool because of its minimal sample consumption, high sensitivity, and short acquisition time. For glycan sequencing, linear or branched oligosaccharides are labeled with a mass tag reagent and analyzed by positive-ion electrospray ionization with tandem mass spectrometry (ESI-MS/MS). Under low energy collision-induced dissociation (CID), the oligosaccharides provide fragments which have information about the glycan structure.Free radical initiated peptide sequencing (FRIPS) produces the similar results obtained by electron capture dissociation (ECD) technique through collision-induced dissociation (CID). The FRIPS demands the introduction of a free-radical generation group into an analyte so that a radical species can be generated under CID conditions.In our previous study, we have designed and synthesized a new tag reagent which is based on 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) radical. Furthermore, we have synthesized a tag reagent containing a new fluorescent structure in addition to the TEMPO moiety so that the mass tag allows FRIPS-MS analysis with easy detection ability during the chromatography.

Poster Presentation : **ORGN.P-376**

Organic Chemistry

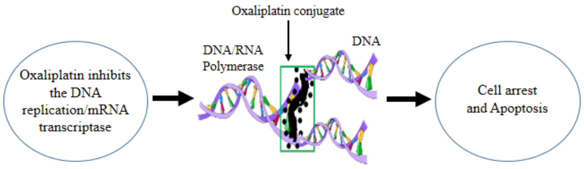
Exhibition Hall 1, FRI 11:00~12:30

Functionalized Novel Cell-Penetrating Peptide-mediated Platinum Conjugate for Cancer Therapy

Tejinder Singh, Akula Murthy, Jungkyun Im*

Department of Chemical Engineering, Soonchunhyang University, Korea

In spite of the research and development of a large number of novel antitumor drugs over the decades, cancer remains one of the most common fatal diseases in humans, worldwide. The conventional anticancer drugs have been encountered with many drawbacks, for instance, high cytotoxicity, lack of target specificity, and very short serum half-life. Cisplatin and some of its platinum complexed derivatives are among the most active anticancer therapeutic agents. Unfortunately, applications of the platinum derivatives always exhibit adverse drug reactions. Therefore, through rational drug design, we have developed a novel cell-penetrating peptide (CPP) and platinum drug conjugate, to overcome previously mentioned issues. Cell-penetrating peptide facilitates intracellular delivery of various cargos through diverse pathways and acts as a delivery vehicle. MTT assay confirmed that the survival rate of cancer cell lines and the resulting IC_{50} values of the conjugate were much reduced than those of parent drug. Cellular internalization was observed by confocal microscopy, which has confirmed that the conjugate was well internalized. Our data demonstrate that CPP-mediated platinum conjugate is very promising and efficient for cancer therapy.



Oxaliplatin Mechanism of Action

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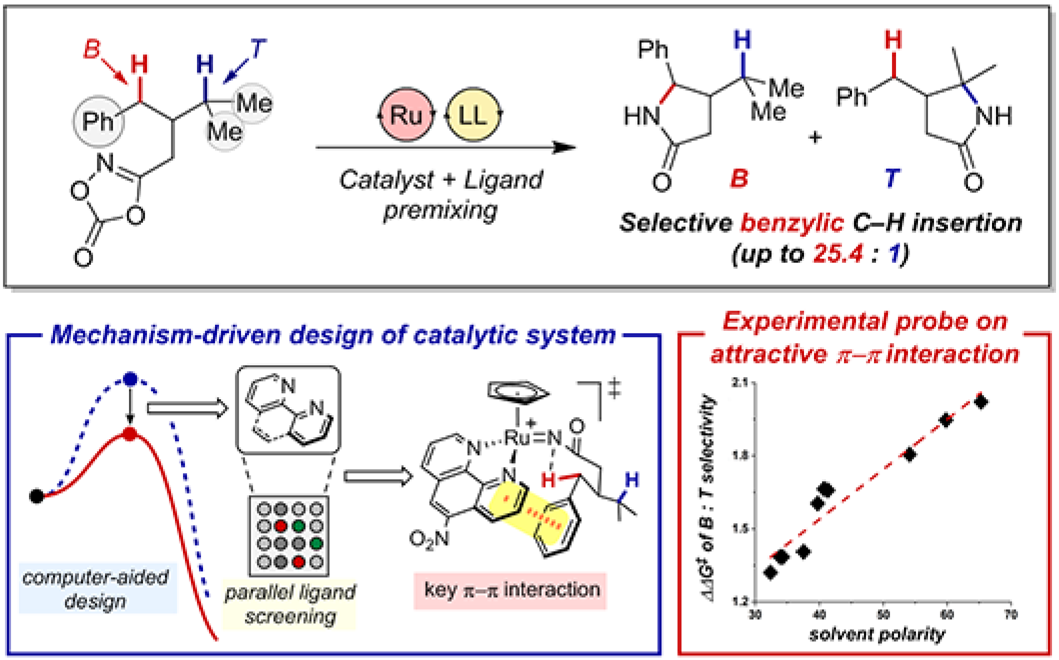
Poster Presentation : **ORGN.P-377**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Harnessing Secondary Coordination Sphere Interactions Enables the Selective Amidation of Benzylic C−H Bonds

Hoimin Jung, Malte Schrader[1], Dongwook Kim[2], Mu-Hyun Baik[*], Yoonsu Park[*], Sukbok Chang[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster, Germany*
[2]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

Engineering site-selectivity is highly desirable especially in C−H functionalization reactions. We report a new catalyst platform that is highly selective for the amidation of benzylic C−H bonds controlled by π-π interactions in the secondary coordination sphere. Mechanistic understanding of the previously developed iridium catalysts that showed poor regioselectivity gave rise to the recognition that the π-cloud of an aromatic fragment on the substrate can act as a formal directing group through an attractive non-covalent interaction with the bidentate ligand of the catalyst. Based on this mechanism-driven strategy, we developed a cationic (η^5-C_5H_5)Ru(II) catalyst with a neutral polypyridyl ligand to obtain a record-setting benzylic selectivity in an intramolecular C−H lactamization in the presence of tertiary C−H bonds at the same distance. Experimental and computational techniques were integrated to identify the origin of this unprecedented benzylic selectivity, and robust linear free energy relationship between solvent polarity index and the measured site-selectivity was found to clearly corroborate that the solvophobic effect drives the selectivity under Curtin-Hammett control. The generality of the reaction scope and applicability towards versatile γ-lactam synthesis were demonstrated.


B
H
H
T
Ph
Me
Me
N
O
O
O
Ru
LL
Catalyst + Ligand premixing
Ph
H
HN
Me
Me
O
B
+
H
Ph
NH
T
O
Selective benzylic C–H insertion (up to 25.4 : 1)
Mechanism-driven design of catalytic system
computer-aided design
parallel ligand screening
N
N
Ru
N
O
N
N
H
H
O_2N
‡
+
key π–π interaction
Experimental probe on attractive π–π interaction
ΔΔG‡ of B : T selectivity
2.1
1.8
1.5
1.2
30
40
50
60
70
solvent polarity

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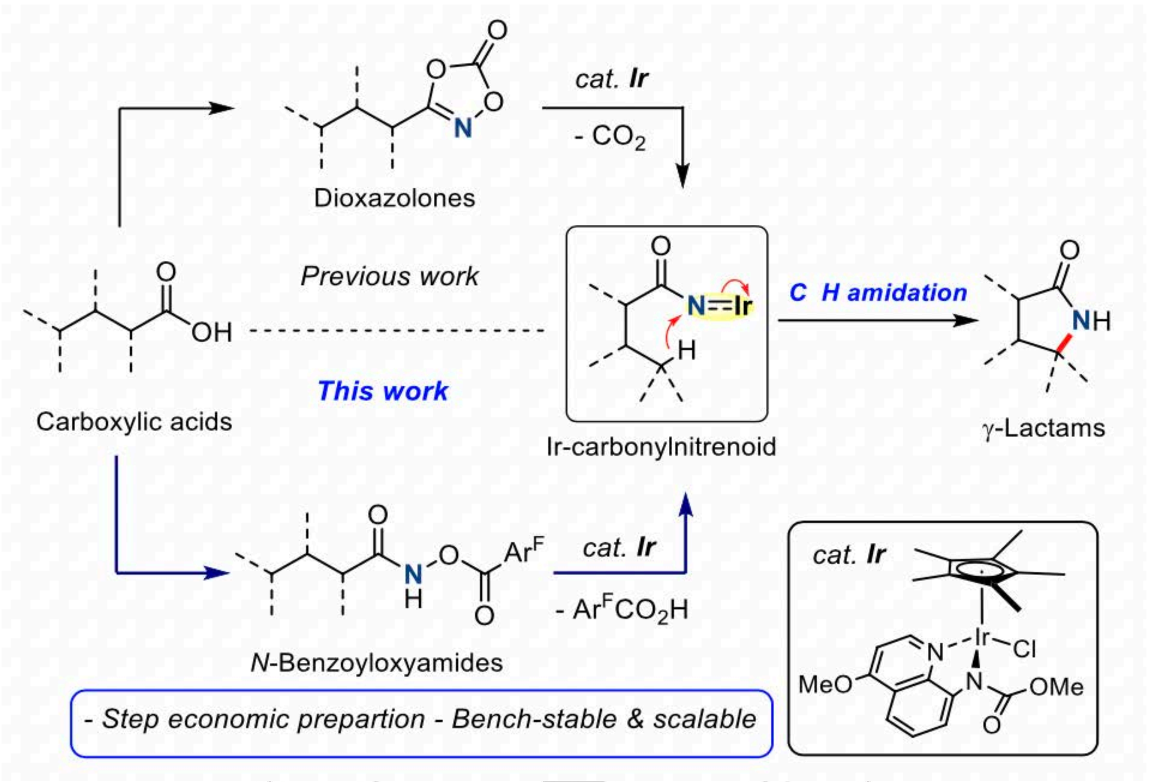
Poster Presentation : **ORGN.P-378**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthetic Utility of N-Benzoyloxyamides as an Alternative Precursor of Acylnitrenoids for γ-Lactam Formation

Soohee Huh, Seung Youn Hong, Sukbok Chang*

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

Cyclic amides are ubiquitous in alkaloid natural products and biologically active compounds. In particular, γ-lactams are a privileged scaffold being widely present in important pharmaceutical agents. Therefore, the development of efficient and selective synthetic routes to this 5-membered amide starting from readily available compounds is of great interest.Recently, we showed that (pentamethyl)cyclopentadienyl (Cp*)-based Ir complexes with engineered bidentate ligands display an unprecedented performance in catalytic C−H amidation of dioxazolones with effective suppression of such side pathway. Herein, we present a new entry of acylnitrenoid precursors for γ-lactam synthesis via an intramolecular C−H amidation reaction. Upon the action of Ir catalysis, N-benzoyloxyamides serve as efficient substrates to afford 5-membered amides. Mechanistic studies revealed that the generation of a putative Ir-carbonylnitrenoid via N−O bond cleavage is facilitated by the chelation of counter cations. This protocol offers a convenient and step-economic route to γ-lactams starting from the corresponding carboxylic acids.


cat. **Ir**
- CO_2
Dioxazolones
Previous work
This work
Carboxylic acids
OH
N=Ir
H
Ir-carbonylnitrenoid
C H amidation
NH
γ-Lactams
Ar^F
cat. **Ir**
- Ar^FCO_2H
N-Benzoyloxyamides
cat. **Ir**
Ir
Cl
MeO
OMe
- Step economic prepartion - Bench-stable & scalable

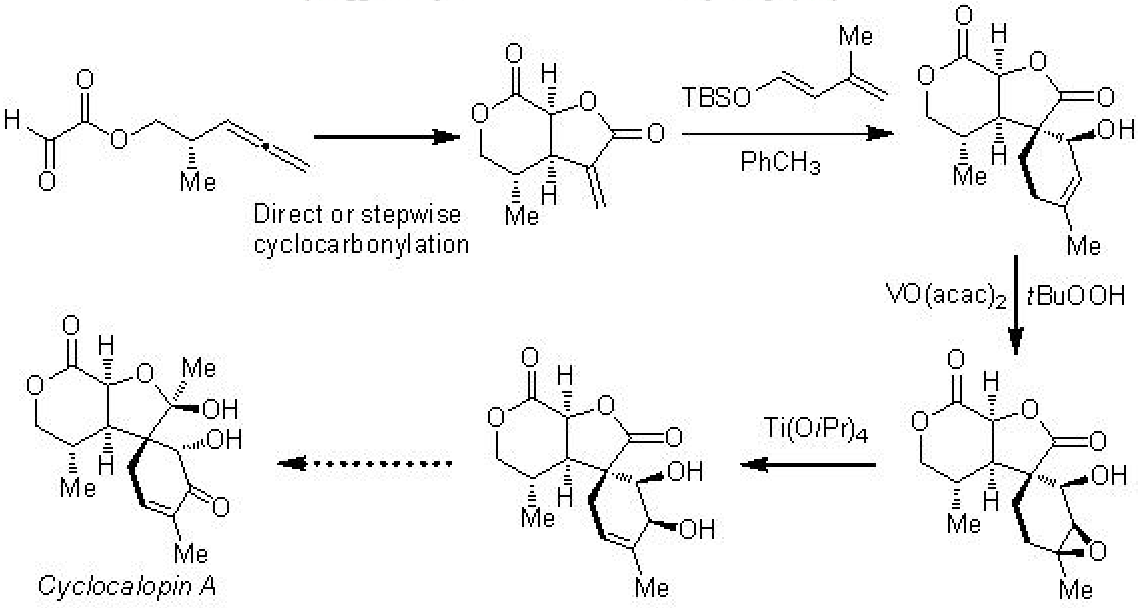
Poster Presentation : **ORGN.P-379**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Construction of Spirosystem of Naturally Occurring Cyclocalopin Family: Toward a Synthesis of (+)-Cyclocalopin E

<u>Weonju Yu</u>, Sehui Yang, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of transition metals are some of the most attractive methodologies since reactions can directly construct complicate molecules from relatively simple starting materials. The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. We developed reaction routes from allenyl glyoxylate to bicyclic lactone in 3 step sequence. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring cyclocalopin series: i. stereoselective elaboration of a spiro-system in cyclocalopin structure; ii. synthetic approach to cyclocalopin family.



Poster Presentation : **ORGN.P-380**

Organic Chemistry

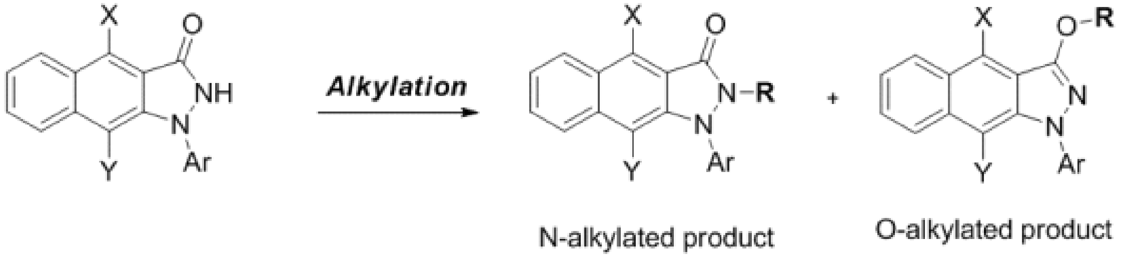
Exhibition Hall 1, FRI 11:00~12:30

Studies on the selective N- or O-alkylation of 1-phenylbenzo[f]indazol-3-one and its biological evaluation

Hyunjin Lee, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Indazolone is known as an interesting chemical moiety because of its importance for the synthesis of a variety of physiologically active compounds. Previously we have synthesized various 1-substituted benzo[f]indazol-3-one derivatives for pharmaceutically important compounds and found that there is a certain tendency between the structure of its derivatives and biological evaluation. The difficulty often encountered in the alkylation of 1-substituted indazolone compounds is that O-alkylated and N-alkylated products are formed simultaneously. In order to further investigate the structure-activity relationship (SAR) between O-analog and N-analog, there is a need to develop a highly selective synthesis method for N-alkylated or O-alkylated compounds. However, there have been no reports on the O- and N-alkylation of pyrazolones to date. Thus, we needed to study the factors that can control the ratio of O- or N-alkylated adducts. Herein, we report optimal conditions for the selective synthesis of O- or N-alkylated adducts in the alkylation of 1-phenylbenzo[f]indazol-3-one derivatives. Oxidation of N-alkylated or O-alkylated intermediate gave the corresponding naphthoquinone-type indazol-3-ones or 3-alkoxypyrazoles. It was observed that their biological evaluation showed potent anti-inflammatory activities.



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Poster Presentation : **ORGN.P-381**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

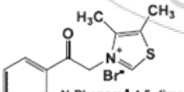
Synthesis and biological evaluation of various 2-naphthalenacetyl thiazolium salts as potential AGEs breakers

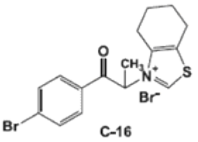
Hakwon Kim[*], JiSue Lee

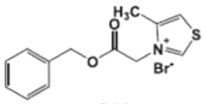
Department of Applied Chemistry, Kyung Hee University, Korea

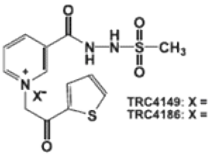
Advanced glycation end products, namely AGEs, are proteins or lipids that become glycated as a result of exposure of sugars. They can be a factor in aging and in the development or worsening of many degenerative diseases, such as diabetes, atherosclerosis, chronic renal failure, and Alzheimer’s diseases. Compounds that are thought to break some existing AGE crossllinks include Alagebrium (ALT-711). N-Phenyl acetyl thiazolium salt, a core structure of alagebrium, could be synthesized from the reaction of N-phenyl acetyl halide and thiazole. But, to date, no drug for AGEs breaking has been developed.In this work, we have synthesized various novel acetyl-4,5-dimethylthiazolium salts bearing naphthalene moieties, such as naphthalene analogs of alagebrum. Those are prepared from various 2-haloacetylnaphthalene derivatives which were synthesized via several routes. Those were tested for AGE breaking.

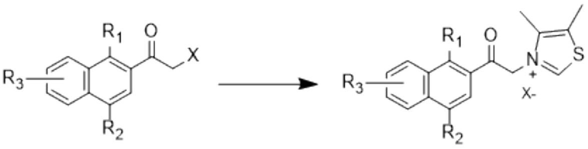

N-Phenacyl-1,3-thiazolium bromide (PTB)


N-Phenacyl-4,5-dimethyl-1,3-thiazolium bromide
ALT-711, Alagebrium


C-16


C-36


TRC4149: X = Br
TRC4186: X = Cl



Poster Presentation : **ORGN.P-382**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Development of new near-infrared emitting benzorhodamine dyes

Mingchong Dai, Kyo Han Ahn[1,*]

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

Rhodamines have been widely used as fluorescent probes and laser dyes because they have high fluorescence quantum yields, high absorption coefficients as well as good photostability. They are also used for studying structure and dynamics of micelles and single-molecule imaging in live cells.[1]. Most of the rhodamine derivatives have very small Stokes shifts. To minimize cross-talk between the excitation source and the fluorescent emission in cellular imaging with high signal-to-noise ratio, large Stokes shifts (typically over 80 nm) are needed.[2] Also, they absorb and emit below 600 nm, rather shorter wavelength absorption and emission wavelengths, which can cause significant autofluorescence from intrinsic biomolecules such as riboflavins and others in tissue imaging. To alleviate those potential drawbacks of rhodamine dyes, we have designed and synthesized a new series of linear and bent shaped benzorhodamine derivatives, which have one additional benzene ring to the rhodamine xanthene core. These new dyes emit in the orange (~600 nm in the case of bent shaped derivatives) and NIR (~750 nm in the case of linear shaped derivatives) regions in aqueous media. These dyes also have good solubility in aqueous media and exhibit high absorptivity, good optical brightness, moderate photostability, and large Stokes shifts in aqueous media. We anticipate that these new benzorhodamine dyes provide a new scaffold for the development of molecular probes and imaging agents for biological applications.[3]References1 a) X. Chen, T. Pradhan, F. Wang, J. S. Kim, and J. Yoon. Chem. Rev., 2012, 112, 1910–1956; b) H. Zheng, X. Zhan, Q. Bian and X. Zhang. Chem. Commun., 2013, 49, 429-447.2 J. F. Araneda, W. E. Piers, B. Heyne, M. Parvez, R. McDonald, Angew. Chem., Int. Ed., 2011, 50, 12214−12217.3 M. Dai et al, manuscript under submission.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-383**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of 2-phenylbenzofuran derivatives via Kukhtin-Ramirez-type reaction and photochemical cyclization

Sunjoo Hwang, Won-jin Chung*

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

Substituted benzofuran is one of the most important structural motifs in several bioactive molecules.[1] There have been many efforts to develop efficient synthetic methods for the construction of substituted benzofuran.[1] Herein, we report a new method for 2-phenylbenzofuran derivatve synthesis via a sequence of a Kukhtin-Ramirez-type reaction and a photochemical cyclization. During our study on functionalization of dioxaphospholene, phosphate was formed unexpectedly via dealkylation.[2] Because it is known that α-keto phosphate can be converted into 2-phenylbenzofuran under photochemical conditions,[3] the combination of these two process led to development of a new synthetic method. With this strategy, 2-phenylbenzofuran derivatives can be easily prepared from 1,2-diketone.

References

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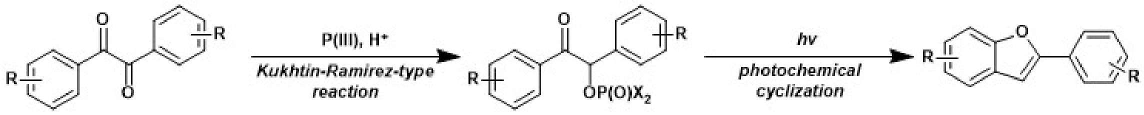
2. Kluger, R.; Taylor, S. D. *J. Am. Chem. Soc.* **1991**, *113*, 996-1001.
3. Givens, R. S.; Athey, P. S.; Matuszewski, B.; Kueper, L. W., III.; Xue, J.-y.; Fister, T. *J. Am. Chem. Soc.* **1993**, *115*, 6001-6012.



Poster Presentation : **ORGN.P-384**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Indole Derivatives in a Continuous Flow Reactor under Mild Conditions

Sumin Nam, Chan Pil Park*

Graduate school of analytical science &technology, Chungnam National University, Korea

Indole-3-carboxyaldehyde synthesized by C3-formylation of indole has various biological activities and is also used as a precursor for synthesizing useful indole derivatives by helping indole functionalization. The methods developed so far have problems such as the use of strong acids and strong bases, the use of metal catalysts and long reaction times. In this study, C3-formylation of indole occurs using Hexamethylenetetramine(HMTA) as carbon source and mild iodine molecule as catalyst. However, this reaction takes a long reaction time in the batch and has a problem of low yield compared to the reaction time. To improve the problem, the microreactor was applied to optimize various parameters. As a result, at 140℃, the yield was 76% in 10 minutes. At 150℃ and 160℃, the yield was 79% in 8 minutes. Especially, at 160℃, the yield was 77% in 5 minutes. Therefore, the problem was solved by reducing the reaction time from 10 hours in a batch to 5 minutes using the microreactor.

Poster Presentation : **ORGN.P-385**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

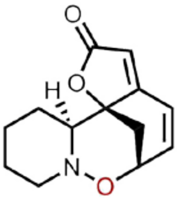
Syntheses of Oxidized *Securinega* Alkaloids

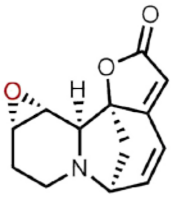
Gyumin Kang, Sanghyeon Lee, Hee-Yoon Lee[*], Sunkyu Han[*]

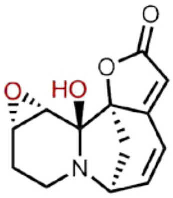
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

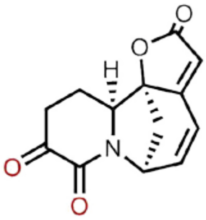
Securinega alkaloids have attracted synthetic community due to their characteristic bridged tetracyclic structure and diverse bioactivities and served as a testing ground of novel synthetic methods. Recently, various *Securinega* alkaloids with higher oxidation state bearing additional carbons unit were isolated, showing diverse structure and potential bioactivities. In order to investigate their intriguing chemistry, we have developed methods for a regioselective oxidation of *Securinega* alkaloids and their further derivatization. Furthermore, application to syntheses of oxidized *Securinega* alkaloids is presented.

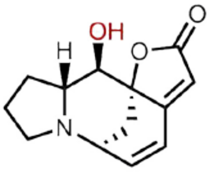
Oxidized *Securinega* Alkaloids with Added Oxygen(s) / Rearranged skeleton

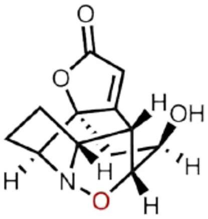

phyllantidine

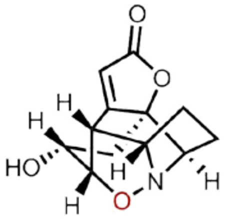

securigine C

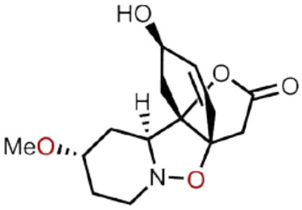

securigine D


securigine E

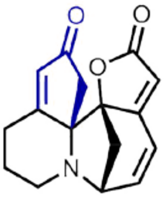

secu'amamine A

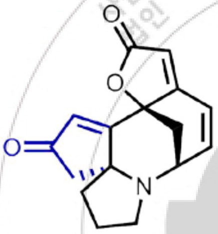

virosaine A

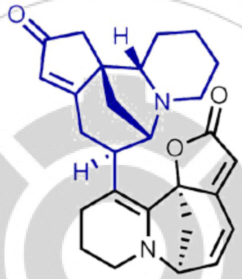

virosaine B

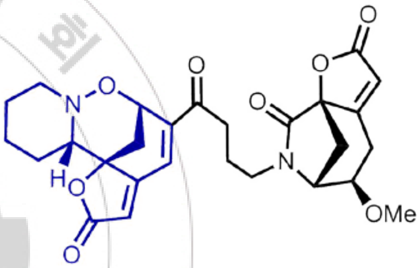

securigine A

Oxidized *Securinega* Alkaloids with Added Carbon Unit / Rearranged skeleton


fluvirosaone A


fluvirosaone B


flueggeacosine A


flueggeacosine B

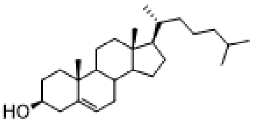
Poster Presentation : **ORGN.P-386**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and biological evaluation of cholestenol, cholestenol amine and their hydrophilic derivatives

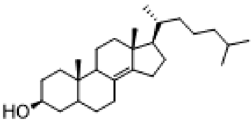
Hyejin Moon, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

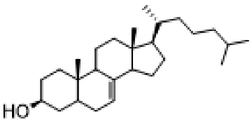
Natural spinasterol-glucose (3-O-β-D-glucopyanosylspinasterol), isolated from *Stewartia koreana* leaves, was identified as a potent anti-inflammatory compound. One wanted to do more research on spinasterol glycosdies, but it was difficult because a steroidal backbone, such as spinasterol, was not easily obtained. Therefore, we developed 5,6-dihydroergosterol and $\Delta^{8(14)}$-ergostenol as alternative steroidal scaffolds that could be used in place of spinasterol, and studied the synthesis of their glycoside derivatives and their anti-inflammatory activity. Recently we have found a new sterol, $\Delta^{8(14)}$-cholestenol (Doristerol) and Δ^{7}-cholestenol (Lathosterol) from 7-dehydrocholesterol, which are regioisomers of cholesterol. Pd-catalyzed hydrogenation and subsequent allyllic isomerization of 7-dehydrocholesterol provides $\Delta^{8(14)}$-cholestenol. Δ^{7}-cholestenol was synthesized from the reduction of 7-dehydrocholesterol by Nickel(Ⅱ) Chloride. Also, their azides were prepared by Mitsunobu reaction and the subsequent reduction gave each amine. We have synthesized some hydrophilic $\Delta^{8(14)}$-cholesterol and Δ^{7}-cholestenol derivatives combined with hydrophilic conjugates, such as acids. It was observed that these derivatives showed strong anti-inflammatory activities



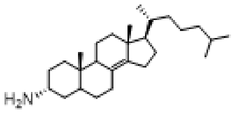
Cholesterol

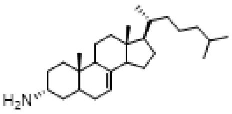


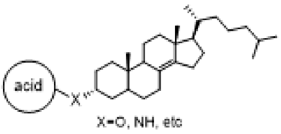
Δ $^{8(14)}$-cholestenol

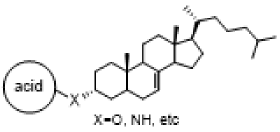


Δ^{7}-cholestenol









Poster Presentation : **ORGN.P-387**

Organic Chemistry

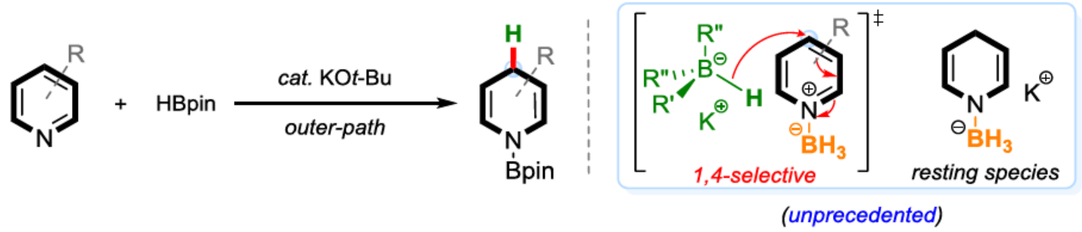
Exhibition Hall 1, FRI 11:00~12:30

Alkoxide-Promoted Selective Hydroboration of *N*-Heteroarenes: Pivotal Roles of in situ Generated BH_3 in the Dearomatization Process

Eunchan Jeong, **Joon Heo**, **Sukbok Chang***

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

While numerous organo(metallic)catalyst systems were documented for dearomative hydroboration of *N*-aromatics, alkoxide base catalysts have not been disclosed thus far. Described herein is the first example of alkoxide-catalyzed hydroboration of *N*-heteroaromatics including pyridines, providing a broad range of reduced *N*-heterocycles with high efficiency and selectivity. Mechanistic studies revealed an unprecedented counterintuitive dearomatization pathway, in which (i) pyridine-BH_3 adducts undergo a hydride attack by alkoxyborohydrides, (ii) in situ generated BH_3 serves as a catalytic promoter, and (iii) 1,4-dihydropyridyl borohydride is in a predominant resting state.



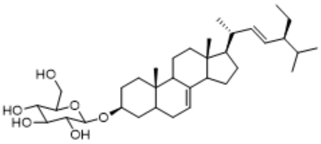
Poster Presentation : **ORGN.P-388**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Biological Evaluation of Cholest-8(14)-en-3-ol and Its Glycosides

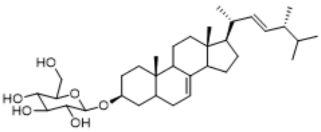
Yeseul Park, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

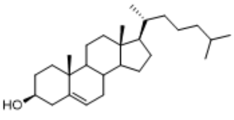
Natural spinasterol-glucose (3-O-β-D-glucopyranosylspinasterol), isolated from *Stewartia koreana* leaves, was identified as a potent anti-inflammatory compound. The activity of Spinasterol or Spinasterol-glucose attracted a great deal of interest, and much research has been done on it, but its separation and synthesis are both difficult, and further research, that is, the development of new drugs, has been difficult. We have therefore developed readily available sterols, such as 5,6-dihydroergosterol and $\Delta^{8(14)}$-ergostenol as analogs of spinasterol. We found that their glycosides showed strong anti-inflammatory activities. In this work, we present the synthesis and biological evaluation of a new sterol, cholestenol (cholest-8(14)-en-3-ol) prepared from 7-dehydrocholesterol, and its glycosides. Pd-catalyzed hydrogenation and subsequent allyl isomerization of 7-dehydrocholesterol provides cholestenol, and Schmidt glycosylation provides the corresponding glycosides according to known literature methods. It was observed that biological evaluation of these glycosides showed strong anti-inflammatory activity.



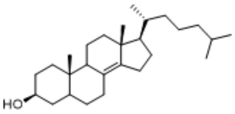
Spinasterol Glucose



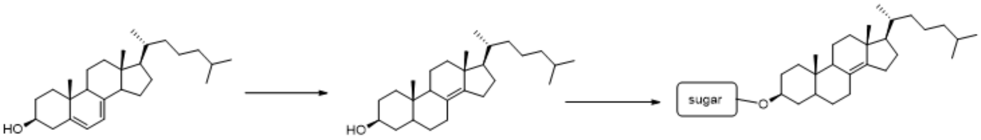
5,6-Dihydroergosterol Glucose



Cholesterol



Cholestenol



7-Dehydrocholesterol

Cholestenol

Cholestenol glycoside

Poster Presentation : **ORGN.P-389**

Organic Chemistry

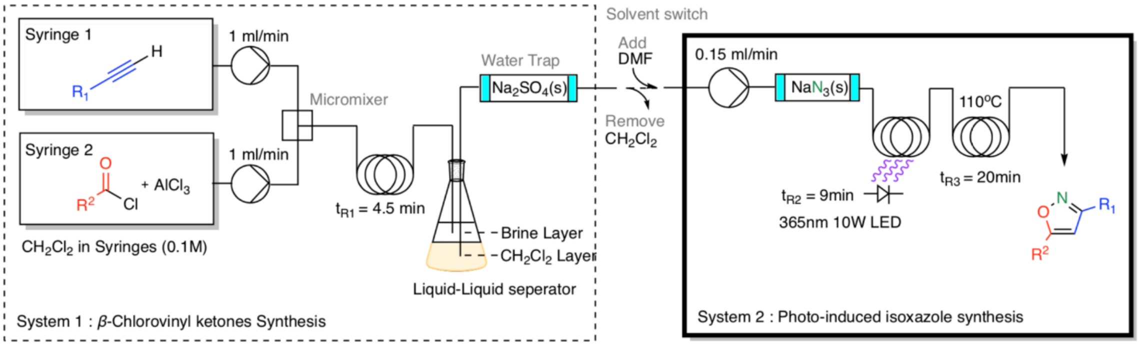
Exhibition Hall 1, FRI 11:00~12:30

A Flow Approach to Synthesis of Isoxazoles

Hyungmo Koo, **Hun Young Kim***, **Kyungsoo Oh***

College of Pharmacy, Chung-Ang University, Korea

We recently developed a selective synthetic method to (*E*)-*β*-chlorovinyl ketones. Continuing the developed flow system, we applied our flow system to the preparation of isoxazoles, a key component of many FDA-approved drugs such as Valdecoxib, Oxacillin, and Cloxacillin. In this presentation, we provide the modular flow system that troubleshoots the side reaction and by-product formation issues. The current multi-step flow system, unlike the batch reaction, can readily modulate the flow synthesis at the point of problems. Thus, our flow module is anticipated to be readily applicable to the synthesis of a variety of heteroaromatic compounds.



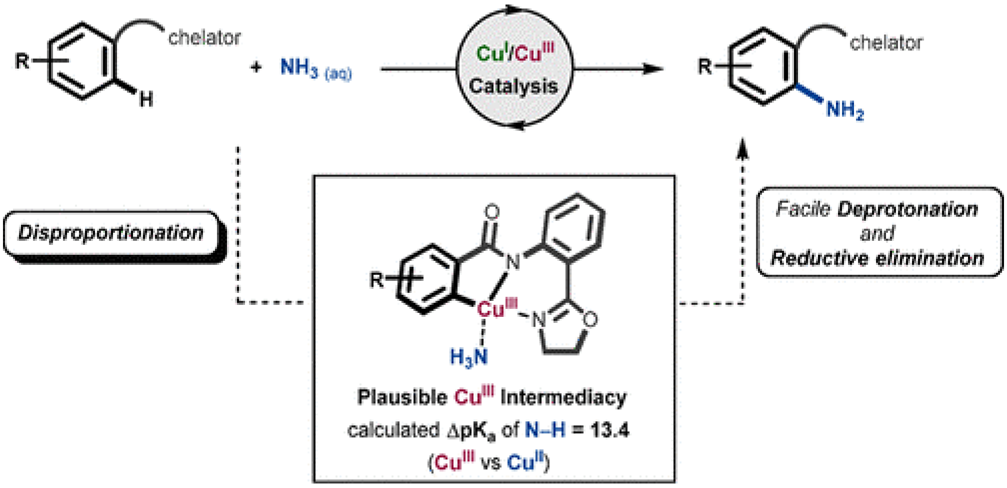
Poster Presentation : **ORGN.P-390**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Copper-Mediated Amination of Aryl C–H Bonds with the Direct Use of Aqueous Ammonia via a Disproportionation Pathway

Joon Heo, Mu-Hyun Baik[1,*], Sukbok Chang[*]

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

The direct amination of C−H bonds with ammonia is a challenge in synthetic chemistry. Herein, wepresent a copper-mediated approach that enables a chelation-assisted aromatic C−H bond aminationusing aqueous ammonia. A key strategy was to use soft low-valent Cu(I) species to avoid the strongcoordination of ammonia. Mechanistic investigations suggest that the catalysis is initiated by a faciledeprotonation of bound ammonia, and the C−N coupling is achieved by subsequent reductiveelimination of the resultant copper−amido intermediate from a Cu(III) intermediate that is readilygenerated by disproportionation of low-valent copper analogues. This mechanistic postulate wassupported by a preliminary kinetic isotope effect study and computations. This new chelation-assisted,copper-mediated C−H bond amination with aqueous ammonia was successfully applied to a broadrange of substrates to deliver primary anilines. Moreover, the mild conditions required for thistransformation allowed the reaction to operate even under catalytic conditions to enable a late-stageapplication for the preparation of pharmaceutical agents.



- Chelation-assisted **C–H amination of arenes** with aqueous **NH_3**
- Intermediacy of **Cu(III)** that enables facile **deprotonation** & **reductive elimination**
- A key **disproportionation** of copper precursor accelerates the reaction
- Copper loading can be lowered to **sub-stoichiometric** amounts

Poster Presentation : **ORGN.P-391**

Organic Chemistry

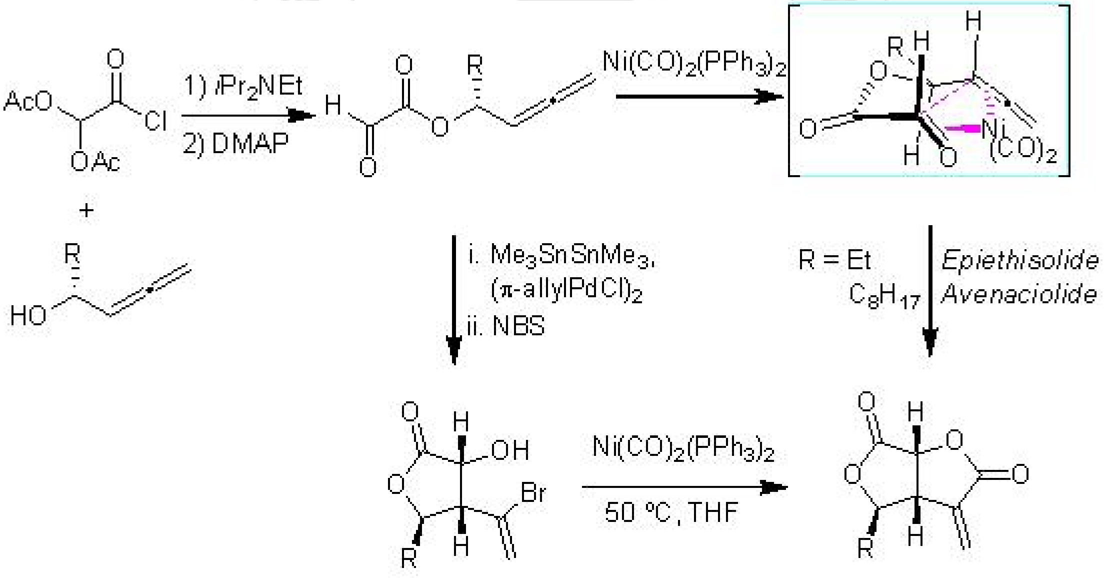
Exhibition Hall 1, FRI 11:00~12:30

Convenient Synthesis of Bioactive Natural Butenolides through Direct or Stepwise Cyclocarbonylation

Jieun Song, Chaofei Wu, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Many organic chemists are attempting to investigate some of these intricate pathways and develop methods to prepare naturally occurring substances in the laboratory. Recently, we set out to investigate a stepwise or direct carbocyclization methods for the synthesis of bicyclic bislactones from allenyl glyoxylates by using transition metals. We would like to present herein several crucial points that have emerged from our recent investigations:1) a novel synthetic method for allenyl glyoxylates 2) direct or stepwise cyclocarbonylation for the synthesis of natural butenolides.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

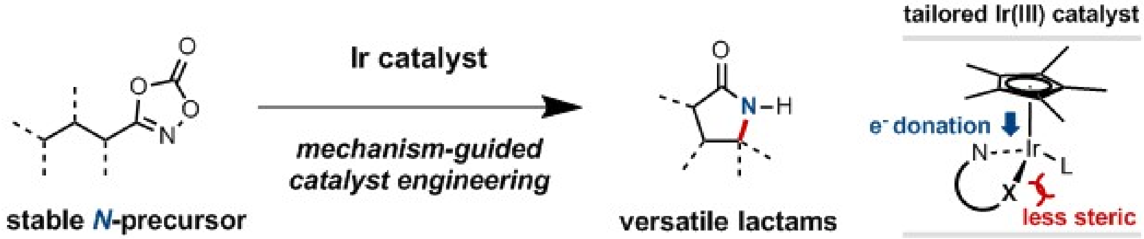
Poster Presentation : **ORGN.P-392**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Nitrene Transfer Reactions for Lactam Synthesis: Catalyst Design, Mechanism and Application

Seung Youn Hong, Sukbok Chang[1,*]

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

Group transfer reactions via metal-nitrenoid intermediate have been emerged as a key strategy to access many heterocycles. Here we present a novel methodology that employs Ir-based catalysts and dioxazolone substrates to access short-lived Ir-nitrenoid complexes, which are key intermediates in the efficient construction of γ-lactams through direct C−H bond amidation. The rational design of efficient and versatile catalysts allows for the straightforward amidations of various sp^3- and sp^2 C−H bonds with exceptional selectivity leading to lactam products. The synthetic utility of this new method is demonstrated in the successful late-stage functionalization of bio-active molecules with amino acid derivatives to produce molecules that are highly sought after for pharmaceutical and other applications in synthesis.We also present an intuitive strategy of ligand participation toward the development of imido transfer into alkyne upon Ir catalysis. Model study reveals that the proposed ligand participation is indeed work via [3+2] cycloaddition to produce a vinyl-lactam Ir species. Moreover, a catalytic haloamidation protocol is also established by employing Ir precatalyst and NaX salts (X = Cl or Br) as a practical halide source to afford synthetically versatile (halovinyl)lactams in excellent *Z*-selectivity. The present mechanistic scaffold was further extended to develop olefin difunctionalization, where putative Ir-nitrenoid is harnessed as a key motif of 1,3-dipoles to enable amido transfer in a *syn*-selective manner. The catalytic reactions provided (haloalkyl)- or (oxyalkyl)lactams in a stereodefined fashion. Product stereochemistry *(threo/erythro)* was found to be designated by the olefin geometry *(E/Z)* of substrates.


stable N-precursor
Ir catalyst
mechanism-guided
catalyst engineering
versatile lactams
tailored Ir(III) catalyst
e⁻ donation
less steric
O
N
H
Ir
L
X

Poster Presentation : **ORGN.P-393**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Oxidatively Induced Reductive Elimination: Exploring the Scope and Catalyst Systems with Ir, Rh, and Ru Complexes

Jinwoo Kim, Dongwook Kim[1], Sukbok Chang[*]

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

Transition-metal catalyzed direct transformation of C–H bonds into carbon-carbon fragments has emerged as a potential alternative to the conventional cross-coupling procedures, providing more straightforward synthetic routes for valuable compounds. In mechanistic viewpoint, among the elementary steps, reductive elimination constitutes a key step for the C–C bond formation and thus extensive studies have been performed to facilitate this process. While conventional low valent pathway suggest thermal reductive elimination, an alternative high-valent pathway in which the oxidation of organometallic intermediate facilitates the C–C bond formation has been appreciated recently for its application on catalytic systems. However, presumably due to the difficulty in the characterization of reaction intermediates, the study on the high-valent pathway has been concentrated on only several species such as Pd, Ni, and Pt catalysts, although direct C–H aryl/alkylation using different metal catalysts also has been actively reported.In this study, we revealed that the *oxidatively induced reductive elimination* (ORE) plays a critical role in C–H aryl/alkylation with Cp^*Ir^{III}, Cp^*Rh^{III}, and (p-cymene)Ru^{II} catalyst systems. Having identified the post-transmetalation intermediates, and combining stoichiometric experiments, cyclic voltammetry analysis, and computational studies, we proved that metallic oxidation of the intermediates facilitates the reductive elimination by significantly mitigating the energy barrier. In addition, we incorporated this mechanistic understanding into the Ir, Rh, and Ru-catalyzed C–H arylation under mild conditions.

Poster Presentation : **ORGN.P-394**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Chlorinative Ring Contraction of 1,4-Dimethoxyphthalazines

Jeong Kyun Im, Ilju Jeong, Won-jin Chung*

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

Our group has been investigating *N*-halogenation of heterocyclic compounds. While attempting *N*-chlorination of 1,4-dimethoxyphthalazine, unexpected ring contraction took place via a loss of one nitrogen atom to give *N*-chlorophthalimide. Although a few examples of related ring contraction of phthalazine-1,4-dione were reported several decades ago,[1,2,3] this type of denitrogenative ring contraction has never been systematically studied. Moreover, the detailed reaction mechanism is still unknown. The newly developed ring contraction is applicable to a wide range of electronically diverse 1,4-dimethoxyphthalazine derivatives. In addition, a plausible reaction mechanism was proposed on the basis of the observed reaction intermediate.

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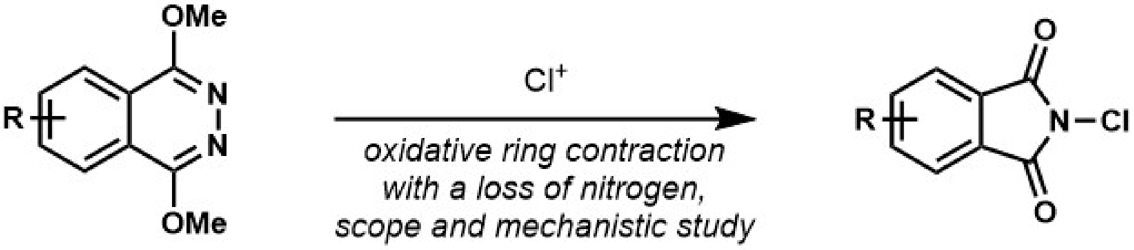


Poster Presentation : **ORGN.P-395**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Abnormal *N*-heterocyclic carbene Pd complexes for copolymerization of ethylene and polar monomers

Da-Ae Park, Ji Yeon Ryu[1], Junseong Lee[1], Sukwon Hong*

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

Functional polyolefins have received much attention in the polyolefin industry due to improved material properties compared to polyolefins. For the synthesis of functional polyolefins, coordination-insertion copolymerization of olefin and polar monomers has emerged as an efficient method to incorporate functional group directly into the polymer chain. However, some challenges remain for incorporating polar monomer into the polymer. Due to the strong σ-coordination of the functional group to the metal, the catalyst results in poor regio- and stereochemistry of polar vinyl monomer insertion, catalyst inhibition and low reaction rates. To overcome these obstacles, the various types of the late-transition-metal catalyst have been developed in copolymerization. The use of *N*-heterocyclic carbenes (NHCs) has become increasingly popular in homogeneous catalysis. Abnormal NHCs (aNHCs) have stronger σ-donating properties than their normal NHCs. We envisioned that aNHC would be appropriate to increase the incorporating ratio of polar monomer into the polymer chain via destabilization of the σ-coordination of functional group on the metal. Herein, we described the synthesis of aNHC-Pd complexes and application in ethylene polymerization and copolymerization with ethylene and polar monomer. The Pd catalysts exhibited good thermal stability and catalytic activity, affording high molecular weight linear polyethylene in ethylene polymerization. Also, the catalytic system allows for good tolerance towards various polar monomers.

Poster Presentation : **ORGN.P-396**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Cryptocyanine-Based Mitochondria-Targeted Photothermogenic Photosensitizer

JaeHyeon Kim, Subin Son, Hyeong Seok Kim, Jiseon Kim, Myung Sun Ji, Jusung An, Ji Hyeon Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Cryptocyanine-based probes exhibit highly efficient photothermal conversion and represent a new class of photothermal agents for use in photothermal therapy (PTT). We have prepared a thermal susceptibility of mitochondria in mind, mitochondria targeted, NIR-absorbing cryptocyanine probe (Mito-CCy) and evaluated its photophysical properties, biological compatibility, photothermal conversion efficiency, cytotoxicity, and mitochondrial localization in HeLa cells. Reactive oxygen species are known to interfere with the mitochondrial defense system and to induce apoptosis. When subject to photoirradiation, Mito-CCy also exhibited high cytotoxicity in HeLa cells by the endogenous production of ROS. The present sensitizer-based photothermogenic approach is rendered more effective by targeting the mitochondria. As such, the system reported here represents the vanguard of what might be a new generation of organelle-targeted photothermal therapeutics.

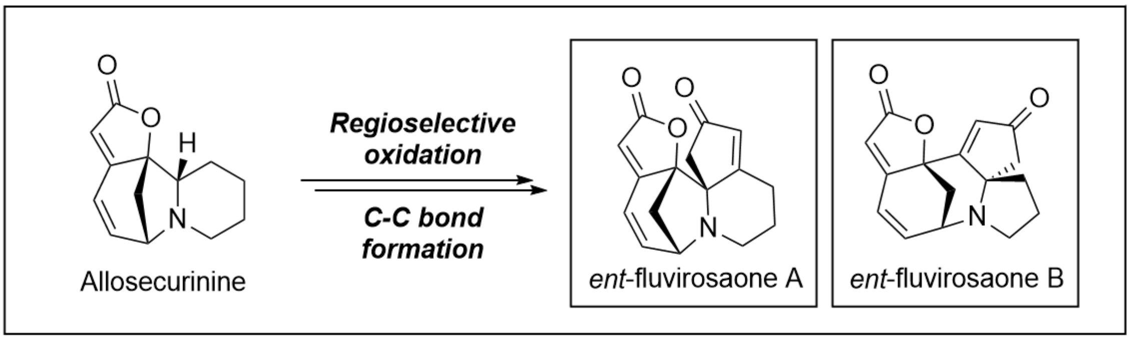
Poster Presentation : **ORGN.P-397**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Bioinspired Total Synthesis of Oxidized *Securinega* Alkaloids:Chemical Insights for the Elucidation of Biogenetic Pathway

Sanghyeon Lee, Gyumin Kang, Sunkyu Han*, Hee-Yoon Lee*

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

For over 60 years, more than 60 *Securinega* alkaloid natural products have been isolated from plants of *Phyllanthaceae* family. Their diverse structure and biological activity have drawn attention from the synthetic community.[1] In 2018, novel type of oxidized *Securinega* alkaloid fluvirosaones A and B were isolated from *Flueggea virosa*. They represent the first pentacyclic *Securinega* alkaloids with three additional carbons unit on the piperidine or pyrrolidine ring.[2]Herein, we present our biogenetically inspired endeavor to ent-fluvirosaones A and B. Discovery of regioselective oxidation of allosecurinine provided the key intermediate for the exploration of the synthetic route to natural products. Skeletal rearrangement of indolizidine core was realized for the first time with *Securinega* alkaloid compound providing new insight for the biogenetic pathways of these natural products...[1] Wehlauch, R.; Grendelmeier, S. M.; Miyatake-O. H.; Sandtorv, A. H.; Scherer, M.; Gademann, K., *Org. Lett.* **2017**, *19*, 548−551.[2] Luo, X.-K.; Cai, J.; Yin, Z.-Y.; Luo, Pan.; Li, C.-J.; Ma, H.; Seeram, N. P.; Gu, Q.; Xu, J. *Org. Lett.* **2018**, *20*, 991–994.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

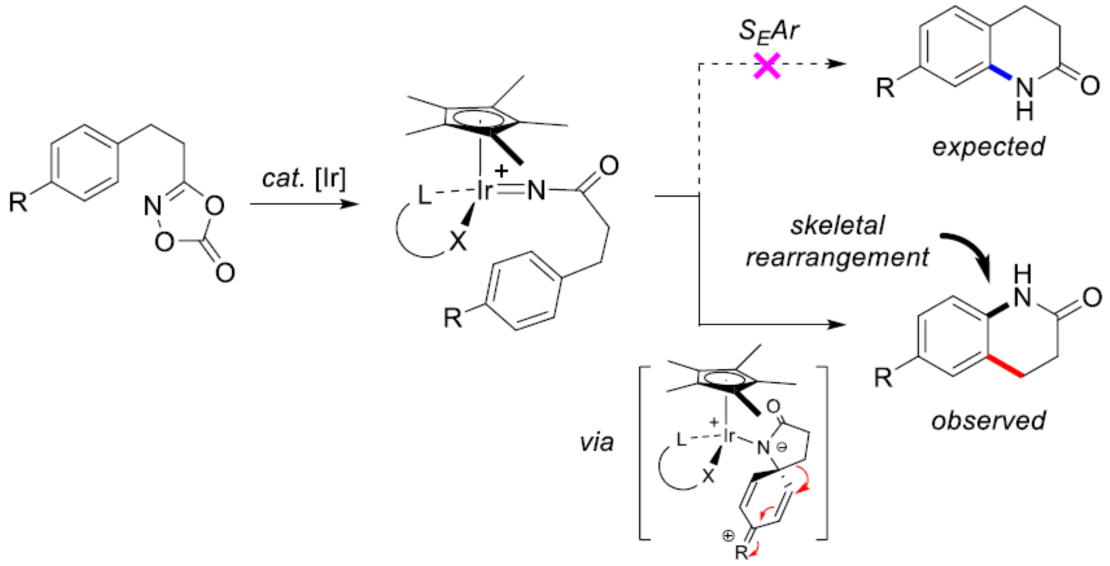
Poster Presentation : **ORGN.P-398**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Revisiting Arene C(sp^2)−H Amidation by Intramolecular Transfer of Iridium Nitrenoids: Evidence for a Spirocyclization Pathway

Yeongyu Hwang, Yoonsu Park, Yeong Bum Kim, Dongwook Kim[1], Sukbok Chang*

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

Two mechanistic pathways, that is, electrocyclization and electrophilic aromatic substitution, are operative in most intramolecular C−H amination reactions proceeding by metal nitrenoid catalysis. Reported here is an alternative mechanistic scaffold leading to benzofused δ-lactams selectively. Integrated experimental and computational analysis revealed that the reaction proceeds by a key spirocyclization step followed by a skeletal rearrangement. Based on this mechanistic insight, a new synthetic route to spirolactams has been developed.



Poster Presentation : **ORGN.P-399**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

1H NMR Chiral Analysis of Chiral Alcohols Enabled by a Gallium-Based Chiral Solvating Agent

Sumin Jang, Hyunwoo Kim[*]

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

The chirality of molecules is an exceptionally important property and a large community in organic chemistry is dedicated to preparing and characterizing chiral molecules for a variety of applications. Chiral high-pressure liquid chromatography (HPLC) and gas chromatography (GC) are the most frequently used methods for chiral analysis. In addition, NMR spectroscopy can be a complementary analytical technique for chiral analysis. Especially with chiral solvating agent, operationally simple and convenient chiral analysis can be accomplished utilizing non-covalent interactions to convert chiral analytes to diastereomeric mixtures. This useful technique was successfully demonstrated for a variety of substrates with chiral amines and carboxylic acids being the most commonly targeted substrates. The emphasis on these species is not surprising, because the majority of chiral solvating agents employ non-covalent interactions such as hydrogen-bonds and electrostatic attractions for structural recognition. Substrates that form relatively weak hydrogen-bonds and are less strongly coordinating such as alcohols are more challenging to study. Here we developed a Ga-based chiral anionic metal complex for 1H NMR chiral analysis of alcohols. Utilizing the optical pKa value, the Ga complex was able to differentiate 1H NMR signals of each (R)- and (S)-enantiomer of alcohols measured at room temperature. Furthermore, this direct 1H NMR chiral analysis of alcohols was used to rapidly determine enantiomeric excess and conversion in a kinetic resolution and an asymmetric synthesis.

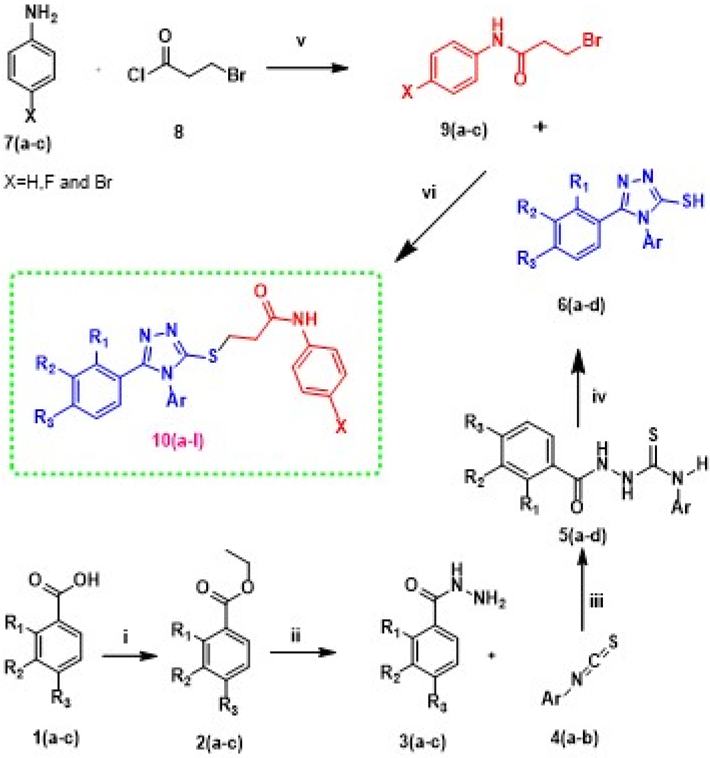
Poster Presentation : **ORGN.P-400**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Biological Evaluation of 4,5 substituted 1, 2,4-Triazoles: A Novel Class of Inhibitors of Mushroom Tyrosinase

Kyou yeong Sim, Balasaheb Daniyal Vanjare[1], Prasad Gajanan Mahajan[1], Nilam Chandrakant Dige[2], Ki Hwan Lee[1,*]

chemistry, Kongju National University, Korea
[1]*Department of Chemistry, Kongju National University, Korea*
[2]*Department of Biological Sciences, College of Natural Science (Building No. 11), Kongju National University, Gongju, Chungnam 32588, Re, Korea*

1,2,4-Triazole derivatives have become progressively attractive to medicinal chemists because of their wide range of biological activities. In this work, different 4 and 5 substituted 1,2,4-triazol-3-ylthio)-N-phenyl propanamide derivatives (10a-l) has been synthesized with good yield and characterized by spectroscopic skills such as LC-MS, 1HNMR, 13CNMR and FT-IR etc. The synthesis was carried out by transforming distinct organic acids into an ester, hydrazides and then 4, 5 substituted 1,2,4-triazole-3-thiol (6a-d). After All, the target compounds (10a-l) were synthesized by the coupling reaction between the para substituted/unsubstituted 3-bromo-N-phenylpropanamide derivatives (9a-c) with the 4, 5 substituted 1,2,4-triazole-3-thiol (6a-d). Moreover, all the synthesized derivatives are tested for mushroom tyrosinase inhibition, the outcomes expose that, all the derivatives display decent results but among all of them, compound 10c (IC50=0.013µM) shows excellent outcome compared with standard drug kojic acid (IC50=16.00 µM).


NH2
X
7(a-c)
X=H,F and Br
O
Cl
Br
8
v
H
N
X
O
Br
9(a-c)
+
vi
R1
N-N
R2
SH
N
R3
Ar
6(a-d)
R1
N-N
O
NH
R2
S
N
R3
Ar
X
10(a-l)
iv
R3
H
S
N
H
N
R2
N
H
R1
O
Ar
5(a-d)
iii
O
OH
R1
R2
R3
1(a-c)
i
O
O
R1
R2
R3
2(a-c)
ii
O
H
N
NH2
R1
R2
R3
3(a-c)
+
S
C
N
Ar
4(a-b)

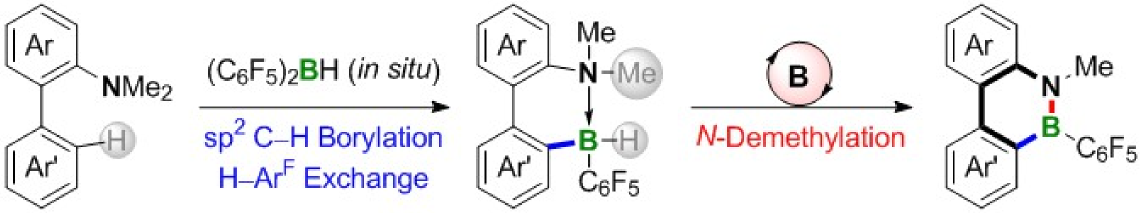
Poster Presentation : **ORGN.P-401**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Sequential C-H Borylation and *N*-Demethylation of 1,1'-Biphenylamines: An Alternative Route to Polycyclic BN-Heteroarenes

Jianbo Zhang, Hoimin Jung[1], Dongwook Kim[2], Sukbok Chang[1,*]

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

Polyaromatic hydrocarbons (PAHs) have drawn great interests in materials chemistry as a key component of organic semiconductors for applications in electronic devices thanks to their unique photophysical and electronic properties being susceptible to molecular structure. In this regard, considerable efforts to substitute the carbon atoms with heteroatoms in the polyaromatic compounds have been made for the invention of new organic materials as isosteres of the parent PAHs with distinctive chemical and electronic properties. Among various isosteres, substitution of a C=C unit with an isoelectronic B-N moiety is one of the most widely studied approaches.An unprecedented access to BN-polyaromatic compounds from 1,1'-biphenylamines via borane-mediated sequential C(sp^2)-H borylation and intramolecular N-demethylation has been developed.[1] The conveniently *in situ* generated Piers' borane from a borinic acid[2] reacts with a series of N,N-dimethyl-1,1'-biphenyl-2-amines in the presence of $PhSiH_3$ to afford six-membered amine-borane adducts bearing a sp^2 C-B bond at the C2'-position. These species undergo an intramolecular N-demethylation by $B(C_6F_5)_3$ catalyst to provide BN-isosteres of polyaromatics. According to computational study, a stepwise ionic pathway is suggested. Photophysical characters of the resultant BN-heteroarenes were shown to be distinctive from those of all-carbon analogues.References[1] J. Zhang, H. Jung, D. Kim, S. Park, S. Chang, *Angew. Chem. Int. Ed.* **2019**, *58*, 7361-7365.[2] a) J. Zhang, S. Park, S. Chang, *Angew. Chem. Int. Ed.* **2017**, *56*, 13757-13761; b) J. Zhang, S. Park, S. Chang, *Chem. Commun.* **2018**, *54*, 7243-7246.



√ *A novel synthetic route to BN-PHAs* √ *Environmetally-benign byproducts* (H_2, CH_4)
√ *First borane-catalyzed N-dealkylation / mechanistically intriguing ionic pathway*
√ *Distinctive photophysical and structural properties of the resultant BN-heteroaromatics*

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Poster Presentation : **ORGN.P-402**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Pd-Catalyzed Regioselective C-H Alkenylation of Azoles Using Alkynes

Woohyeong Lee, Jung Min Joo*

Department of Chemistry, Pusan National University, Korea

Thiazole-containing π-conjugated moieties are important structural units in the development of new electronic and photo-chromic materials. We have developed a palladium-catalyzed *syn*-hydroarylation reaction of diaryl alkynes with thiazoles, which provides access to thiazole-containing triarylethylenes. Pd(II) complexes derived from Pd(0) species and carboxylic acids facilitated C–H functionalization of the unsubstituted thiazole with high C5 selectivity. The catalytic system was also compatible with other azoles, allowing the stereoselective syntheses of various trisubstituted olefins.

Poster Presentation : **ORGN.P-403**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Pd-Catalyzed Synthesis of Strained-Alkene-Fused Heterocycles

Birakishore Padhi, Eunmin Kim, Jung Min Joo*

Department of Chemistry, Pusan National University, India

In continuation of our research interest on C—H functionalization, herein we developed a new palladium-catalyzed strategy for synthesis of a variety of strained alkenes having pyrazole units in a single step. This transformation provides a complex and rigid molecular architecture which will be useful for meterial chemistry, polymer synthesis, and medicinal chemistry research programs. The resulting heteroarene compounds were also further fuctionalized at late stage to provide various types of pyrazole containing compounds.

Poster Presentation : **ORGN.P-404**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Effective HMF Production in the Microreactor System

Yea seul Jang, Chan Pil Park*

Graduate school of Analytical Science & Technology, Chungnam National University, Korea

Recently, many studies have been conducted to preserve the environment. Biomass is receiving much attention as an alternative to protect the environment. Much research has been conducted on the synthesis of HMF (5-hydroxymethylfurfural), a derivative of biomass. In this study, HMF is synthesized through dehydration of fructose under acid catalyst and the optimum conditions for the efficient HMF synthesis using the microreactor were investigated. We studied the reaction time, temperature, solvent composition, and type and amount of catalyst. Also, the method for efficient HMF extraction in the microreactor was considered.

Poster Presentation : **ORGN.P-405**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of Epoxy Alcohols via Tandem reaction in microreactor.

Goeun Son, Chan Pil Park*

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

Epoxy alcohol is used as a building block in organic synthesis, especially, both enantiomeric series are utilized in diverse synthesis. Epoxy alcohols are obtained by oxidation of the allyl group compound in the presence of carbon-carbon double bond. We synthesis the allylic hydroperoxide via photooxygenation of alkenes and to be followed by directly epoxidation without a replacement of reactor, purification. This synthetic method only uses the photosensitizer, oxygen gas to oxidation the allylic compound, is eco-friendly. But longer reaction time, which was a main drawback of the existing reaction. So, we resolve this problem by using the microreactor. this system maximizes the efficiency of photooxygenation by broadening the surface area that receives light, also, is useful to remove the photosensitizer that has an adverse effect on the epoxidation reaction after the photooxygenation. It can be obtained high efficiency, also can be applied to the mass production.

Poster Presentation : **ORGN.P-406**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A new fluorescent sensing platform: self-assembled conjugated polyelectrolyte micelles with amplifying signal transduction

Yeonjin Jang, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Fluorescence-based assays should be feasible in aqueous medium for effective detecting the biological factors. However, numerous sensors have limited signal transductions and low fluorescence quantum yields due to reduced excited state energy of fluorophores inherent in aqueous solution, which leads to reduced sensitivity. Thus, a new smart sensing platform with the amplified fluorescence response for analytes in such an circumstance is still demanding. Herein, a new building block which self-assembles in aqueous media, giving the hydrophobic π-extended conjugated system at the inner part and hydrophilic groups at the periphery, was devised for the first time. We demonstrated that a self-assembly of conjugated units in a micelle provides a channel for efficient energy or electron migration and allows enhanced optical properties, which is a distinct sensing platform from the numerous fluorescence-based tools developed for sensitive detection. This new system exhibited very sensitive signal transduction involving amplified fluorescence quenching in aqueous media.

Poster Presentation : **ORGN.P-407**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

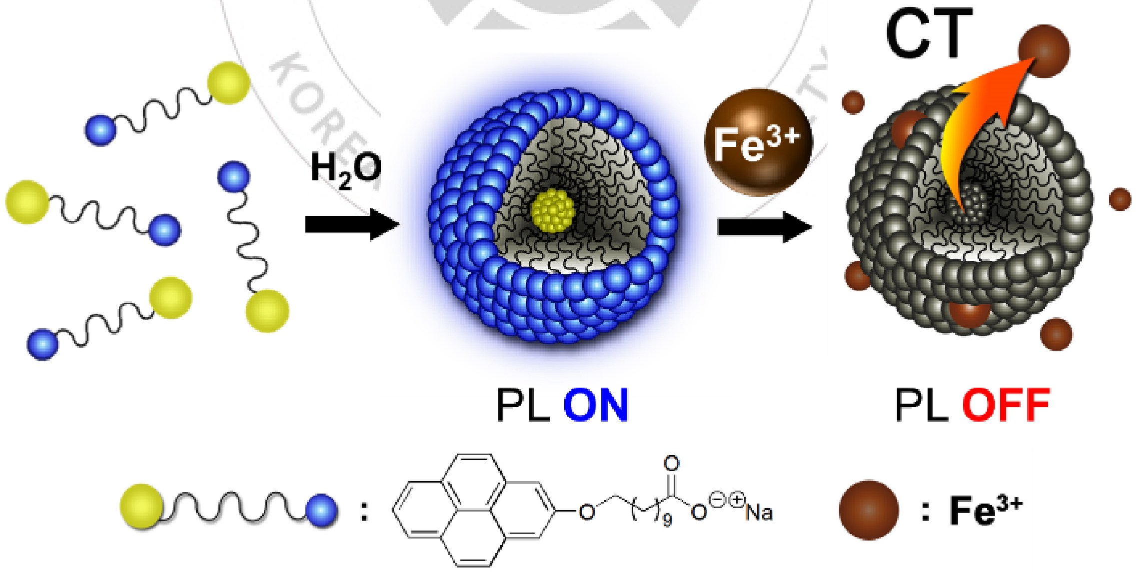
Micellization-induced amplified fluorescence response for highly sensitive detection of NTBI in serum

Tae eun Park, Seoung Ho Lee[1,*]

Department Chemistry, Daegu University, Korea

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

A novel, micelle-based fluorescence system capable of selectively and sensitively signal transduction for non-transferrin bound iron(NTBI) in serum was devised. We demonstrated that an aggregated fluoreginic core in a micelle induces amplified fluorescence quenching, which is a distinct sensing platform from the numerous fluorescence-based tools developed for sensitive detection



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Poster Presentation : **ORGN.P-408**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A ratiometric fluorescence sensor based on enzymatic activatable micellization for quantitative detection of alkaline phosphatase activity

Seoyoon Kim, Jeongmoo Lee[1], Seoung Ho Lee[1,*]

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

A novel ratiometric fluorescence assay via enzymatic activatable micellization in aqueous solution was devised for quantitative detection of alkaline phosphatase activity (ALP). We demonstrated that the dephosphorylation of water-soluble fluorophore 1, which is the phosphate- functionalized monomer, induced by an enzymatic reaction of ALP leads to micelle formation in aqueous solution as its water-soluble functionality reduces. A micellization of 1 by the dephosphorylation exhibits ratiometric sensing response for various ALP concentrations (6-200 mU/mL) and provides a suitable sensing platform for naked eye detection with increased fluorescence quantum yield even compared to known TPE-based sensors, where ALP can be sensed with a detection limit of 0.38 mU/mL. In addition, 1 displays excellent sensing performance at the concentration levels from 0 to 100 mU/mL in human serum, which can provide a capacity to exploit ratiometric responses for real-time assays of bioactive substances.

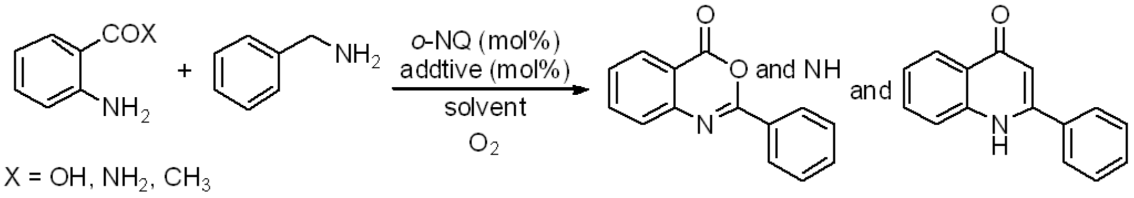
Poster Presentation : **ORGN.P-409**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

o-Naphthoquinone-Catalyzed Cross-Coupling of Amines: A Unified Amine Oxidation Strategy to Heteroaromatic Compounds

Kyeongha Kim, Hun Young Kim[*], Kyungsoo Oh[*]

College of Pharmacy, Chung-Ang University, Korea

Heterocyclic compounds are key constituents in numerous natural products and drug substances, and the development of new synthetic methods to heterocyclic compounds significantly broadens the choice of bioactive compounds that can be targeted. Previously, our group has developed the *ortho*-naphthoquinone-catalyzed aerobic oxidation of amines, where two different amines are cross-coupled to imine derivatives.[1]The utilization of such aerobic oxidation methods has been demonstrated in the synthesis of 3-carboxylic-indoles, where two readily available starting materials, anilines and benzyl amines, were efficiently cross-coupled under the ortho-naphthoquinone-catalyzed aerobic oxidation conditions to the corresponding 2-arylmethyleneaminophenylacetates that in turn smoothly underwent the Cu(II)-catalyzed intramolecular Mannich reaction.[2] Taking initiatives from the previous success in the *ortho*-naphthoquinone-catalyzed amine oxidation strategies, we envisioned the use of aniline derivatives with a diverse functional groups. In this presentation, we report the synthetic approaches to quinazolinones, benzoxazones, and quinolones under the *ortho*-naphthoquinone-catalyzed aerobic oxidation conditions.Reference:1. (a) Goriya, Y.; Kim, H. Y.; Oh, K. *Org. Lett.* **2016**, *18*, 5174-5177. (b) Golime, G.; Bogonda, G.; Kim, H. Y.; Oh, K. *ACS Catal*. **2018**, *8*, 4986-4990.2. Kim, K.; Kim, H. Y.; Oh, K. *Org. Lett.* **2019**, *21*, [doi.org/10.1021/acs.orglett.9b02348]



Poster Presentation : **ORGN.P-410**

Organic Chemistry

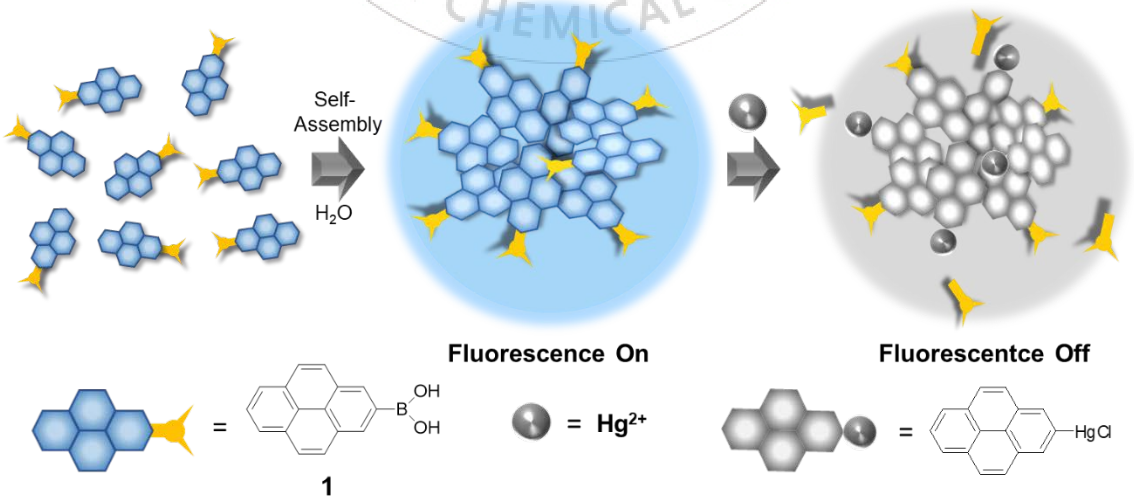
Exhibition Hall 1, FRI 11:00~12:30

Self-assembly of pyrene boronic acid-based chemodosimeters for highly efficient mercury (II) ion

<u>Seung Yeob Lee</u>, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

A new chemodosimeter consisting of pyrene and boronic acid (**1**) for Hg^{2+} ions is described. The amphiphilic nature of **1** leads to self-assembly in aqueous solution and the high electron density throughout the aggregated pyrene units provides an outstanding platform for energy and electron transport. Self-assembled **1** exhibits a selective and sensitive fluorescence response to Hg^{2+} ions where the Hg^{2+} ion allows a fast transmetalation of **1**, which drastically reduces its fluorescence. The Stern-Volmer (SV) quenching constant for the fluorescence quenching of self-assembled 1 by Hg^{2+} ions is about 1.8×10^{6} M^{-1}, and Hg^{2+} ions can be sensed with a detection limit of 6.6×10^{-9} M. In addition, self-assembled **1** exhibits excellent sensing performance at nano-molar concentration levels for Hg^{2+} ion contamination of tap water, fresh water, and seawater.



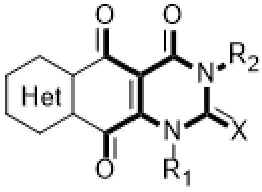
Poster Presentation : **ORGN.P-411**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of benzo[g]quinazoline-2,4,5,10-tetraone derivatives for antibacterial

Kyungmin Kim, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

The synthesis and biological evaluation of quinazoline-2,4-dione and 1,4-naphthoquinone are still considered to have high potential. Therefore, pyrimidine-2,4-dione conjugated with 1,4-naphthoquinone, such as benzo[g]quinazoline-2,4,5,10-tetraone, has attracted a lot of interest to show a potent biological activity. In this study, 3-bromo-1,4-dimethoxy-2-naphthoic acid was used as a starting material to synthesize target materials by amidation, amination, carbonyl addition, and oxidation. We screened the antimicrobial activity against 8 kinds of bacteria including Staphylococcus aureus for new synthetic compounds using minimal inhibitory concentration test (MIC). In addition, we confirmed that antifungal activity against seven fungi including C. albicans. As a result, it was confirmed that one of synthesized samples has excellent antibacterial activity against Staphylococcus aureus.



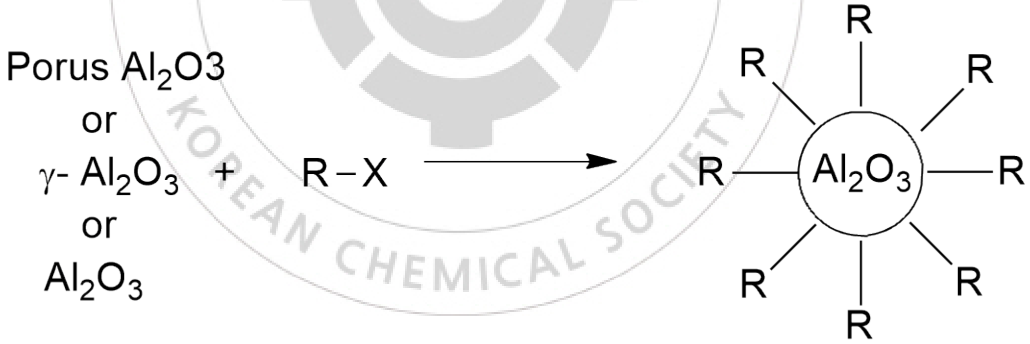
Poster Presentation : **ORGN.P-412**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

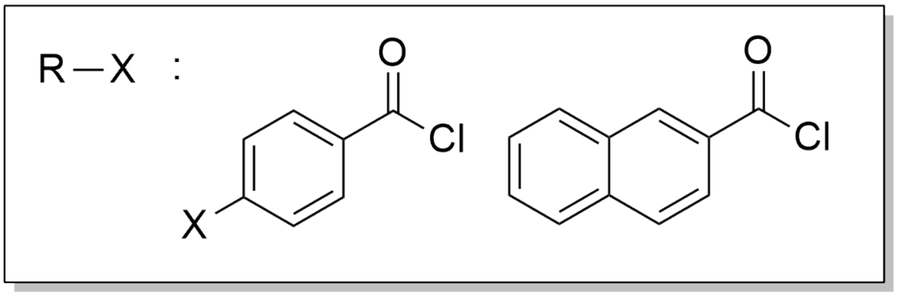
Functionalization of Organic Ligand in Alumina Surface: Photoluminescence Properties

Yongcheol Jung, **Chuljin Ahn***

Department of Biology and Chemistry, Changwon National University, Korea

Although several reactions of phosphoric derivatives with alumina have been reported, the other organic functional groups do not have been used for grafting organic moieties on alumina. In our lab, the hybrid material grafting organic moieties on alumina were prepared through the microwave irradiation or reflux and their photoluminescence (PL) properties were investgated.





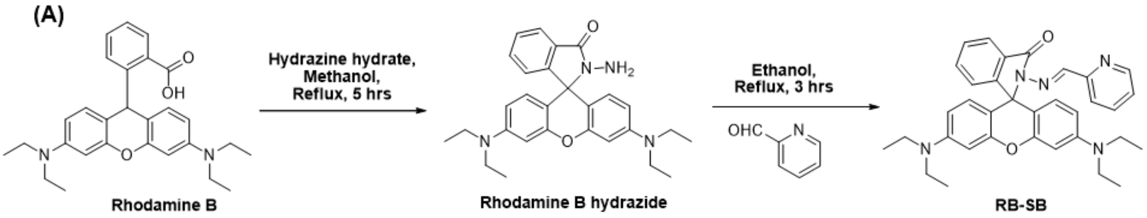
Poster Presentation : **ORGN.P-413**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

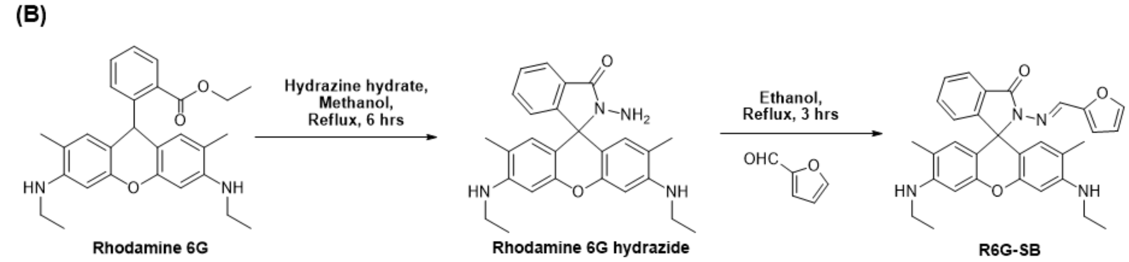
Design, Synthesis and Photophysical properties of Spiro[isoindoline-1,9'-xanthen]-3-ones

Eun hui Song, Chaeeun Lee, Hui Jeong Cho, Prasad Gajanan Mahajan, Balasaheb Daniyal Vanjare, Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

The efficient fluorogenic compounds based on Spiro[isoindoline-1,9'-xanthen]-3-one core has been synthesized in the present study followed by estimation of their photophysical properties in different solvents. The compounds were synthesized through the reaction between rhodamine B/ Rhodamine 6G, hydrazine hydrate and heterocyclic aldehydes. The formation of target compounds was confirmed by spectral techniques such as IR, NMR and Mass analysis. The synthesized compounds were screened for estimation of their different photophysical properties namely absorption maximum, molar extinction coefficient, fluorescence emission maximum, Stokes shift and fluorescence quantum yield in different organic solvents which are of variable polarity nature. The comprehensive comparative study of synthesized compounds and parent molecules (Rhodamine B and Rhodamine 6G) with respect to photophysical properties in different solvents brings significant research output and can be useful to treat these compounds as fluorescent marker and sensors.


(A)
Rhodamine B
Hydrazine hydrate,
Methanol,
Reflux, 5 hrs
Rhodamine B hydrazide
Ethanol,
Reflux, 3 hrs
OHC
RB-SB


(B)
Rhodamine 6G
Hydrazine hydrate,
Methanol,
Reflux, 6 hrs
Rhodamine 6G hydrazide
Ethanol,
Reflux, 3 hrs
OHC
R6G-SB

Poster Presentation : **ORGN.P-414**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Chelation enhanced fluorescence of rhodamine based organic nanoparticles for selective detection of mercury ions in aqueous medium

Jin Sik Shin, Prasad Gajanan Mahajan[1], Nilam Chandrakant Dige[2], Balasaheb Daniyal Vanjare[1], Ki Hwan Lee[1,*]

Department of Chemistry, Chungnam National University, Korea
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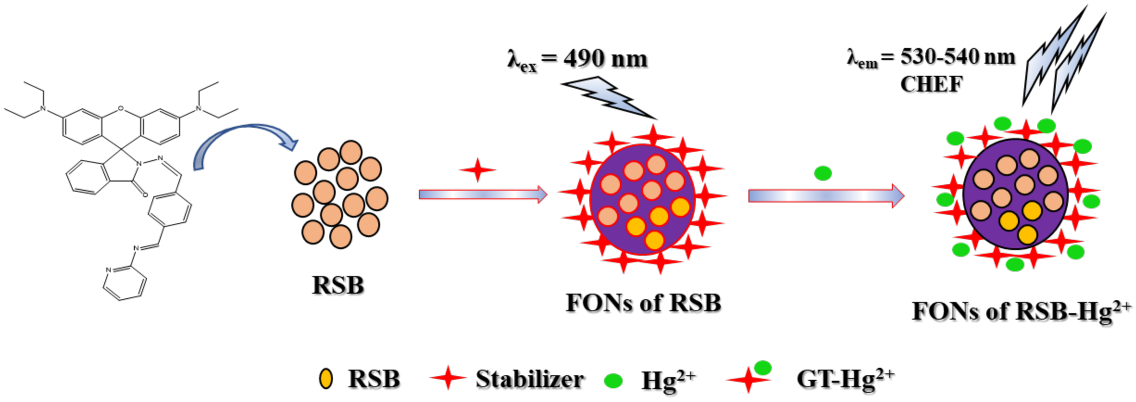
A Schiff base centered fluorescent organic nanoparticles (FONs) were prepared by using rhodamine as structural core (RSB) and a stabilizer. The simple, easy and quick reprecipitation method has been employed for the preparation of FONs of RSB. The formation and morphology of FONs was confirmed by particle size analysis and scanning electron microscopy, respectively. The prepared FONs of RSB found to be more stable and photoactive for the neutral pH. A series of metal ion was used to investigate the change in fluorescence properties of RSB when in contact with and without the target metal ion solutions. Interestingly, only mercury (Hg2+) addition to FONs of RSB shows chelation induced enhanced fluorescence response. While, addition of other metal ions induces negligible fluorescence quenching effect with FONs of RSB. The interaction of FONs of RSB and Hg2+ introduces chelation enhanced fluorescence is unaltered even addition of other metal ion of higher concentration. The studies on UV–vis absorption titration, zeta-particle size, Job's plot and modified Benesi-Hildebrand plot illustrates the strong complexation between FONs of RSB and Hg2+. Thus, such sensing properties posed by prepared FONs will open a simple and quick detection method for hazardous Hg2+ in an aqueous solution. The present analytical approach is advantageous over the traditional analysis methods.


λex = 490 nm
λem = 530-540 nm
CHEF
RSB
FONs of RSB
FONs of RSB-Hg2+
RSB
Stabilizer
Hg2+
GT-Hg2+

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Poster Presentation : **ORGN.P-415**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Development and Biological activity evaluation of saccharin Derivatives from N-hydroxymethyl saccharin

Seung ryul Lee, Do hun Lee, Eon Jin Lee, Dai Il Jung*

Department of Chemistry, Dong-A University, Korea

Saccharin is an artificial or non-nutritive sweetener. Humans can't break down saccharin, so it leaves the body unchanged. Alkylation methods for preparing N- and O-substituted (carbonyl oxygen) derivatives of 1,2-benzisothiazol-3-one-1,1-dioxide (saccharin) are well established, and these have provided researchers with the straightforward synthesis of novel and potentially bioactive molecules. In addition to N- and O-alkylation, compounds modified in the attached benzene ring are particularly preferred. All types of saccharin derivatives attract very intensive interest in the development of new biologically active and small molecule medicines. We have developed promising derivatives of saccharin via esterification from hydroxymethyl saccharin with acyl chloride(stearoyl chloride, lauroyl chloride, decanoyl chloride, heptanoyl chloride, caproyl chloride, octanoyl chloride, hydrocinnamoyl chloride, etc) and will perform biological activity evaluation of the derivatives.

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Poster Presentation : **ORGN.P-416**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Radical Fluorination and 1,2-Alkyl Migration Cascades of Vinyl Cyclobutanols: Synthesis of Fluoromethyl-Substituted Cyclopentanones

Juhee Kim, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A radical fluorination/1,2-alkyl migration cascade process of alkenyl cyclobutanols was developed in this study. This approach provides a mild and convenient access to the synthesis of fluoromethyl-substituted cyclopentanone derivatives from the coupling reaction of alkenylcyclobutanols with Selectfluor as the fluorine radical source.

Poster Presentation : **ORGN.P-417**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis of 3-selenylated imidazo[1,2–α]pyridines using electrochemical oxidation

Juhee Lee, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

Electrochemical oxidative selenylation of imidazo[1,2–α]pyridines has been developed. The reaction proceeds in an undivided electrochemical cell equipped with glassy carbon electrodes employing $LiClO_4$ as a supporting electrolyte. This approach is environmentally benign by using shelf-stable diselenides as selenium source and electrons as oxidizing reagents. The present protocol offers a facile way to prepare β-selenylated imidazopyridine derivatives.

Poster Presentation : **ORGN.P-418**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Photoredox-Catalyzed Selenylation/Ring-Expansion Cascades of Alkenyl Cyclobutanols: Synthesis of β-Selenylated Cyclopentanones

Hyeim Jeong, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

A photoredox strategy to access β-selenated cyclic ketone derivatives through the coupling reaction of 1-(1-arylvinyl)cyclobutanols with diselenides under blue LED irradiation and an air atmosphere was developed. This reaction employs the easily accessible and shelfstable diselenides as a selenium radical source, and the reaction has advantages of mild reaction conditions and broad substrate scope.

Poster Presentation : **ORGN.P-419**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis of β-CF$_3$-substituted ketones via electrochemical trifluoromethylation/1,2-carbon migration sequences of alkenyl alcohols

Hyeim Jeong, Dae Young Kim*

Department of Chemistry, Soonchunhyang University, Korea

Electrochemical oxidative radical trifluoromethylation/semipinacol rearrangement sequences of alkenyl alcohols were developed in this study. This approach is environmentally benign and uses the shelf-stable Langlois reagent as a trifluoromethyl radical precursor and electrons as the oxidizing reagents. The present protocol offers a facile route to prepare β-trifluoromethylated ketone derivatives.

Poster Presentation : **ORGN.P-420**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Synthesis and characterization of liquid crystaillne epoxy containing cyano biphenyl moieties as a mesogen

Soyeong Choe, Hyeonuk Yeo[1,*]

Department of Chemistry, Kyungpook National University, Korea

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

These days, devices such as laptops, smartphones, and AirPods are having more function and smaller in size to make our life easier. Because of these properties, heat from the devices has increased, which reduces the reliability of the device. Therefore, there is a need for a heat dissipating material that efficiently transfers the generated heat. In the materials as a matrix, a liquid crystal epoxy resin (LCER) having strong adhesion to the inorganic filler is often selected. In this research, we tried synthesizing a new liquid crystal epoxy resin having cyano biphenyl (CBs) structure as a mesogen. The synthetic procedures were conducted in two step reactions. In the first reaction, the intermediate compounds, terminal bromoalkoxy-(1,1'-biphenyl)-4-carbonitrile, were synthesized using S_N2 reaction between 4'-hydroxy-(1,1'-biphenyl)-4-carbonitrile and terminal dibromoalkane (carbon number, n=4,5,6,7,8,9). Next reactions were carried out by substitution reaction of the intermediates to glycidol to obtain epoxy monomers with various alkyl linkages. The final compounds were characterized by ^1H NMR analysis. The differential scanning calorimetry (DSC) and polarized optical microscope (POM) were used to investigate their liquid crystalline properties. In DSC measurements, the curves showed heat flow changes at specific temperatures that occurred as phase transitions from solids to liquid crystals and from liquid crystals to isotropic liquids. And the liquid crystal phases could be observed by POM analysis. The details will be presented.

Poster Presentation : **ORGN.P-421**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Electrogenerated chemiluminescence probe for glutathione based on cyclometalated Ir(III) complex

Hyun Seung No, Taemin Kim[1], Jong-in Hong[1,*]

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

Electrogenerated chemiluminescence probe for glutathione based on cyclometalated Ir(III) complexHyun Seung No, Jong-In Hong*Department of Chemistry, Seoul National University, Seoul 08826, KoreaGlutathione (GSH) is the most abundant intracellular biothiol and plays a critical role as a cellular antioxidant. Abnormal levels of GSH are associated with many diseases. Therefore, various detection methods for GSH have been developed. It is challenging to detect GSH selectively among structurally similar biothiols (Cys, Hcy). Recently, an iridium complex ligated with phenanthroline-dione was developed to detect GSH using redox chemistry. Electrogenerated chemiluminescence (ECL) has received much attention due to advantages such as high sensitivity, no light source, simple analytical process, and applicability to point-of-care testing. Herein, we report ECL chemodosimetric probe for GSH based on cyclometalated Ir(III) complexes having a phenanthroline-dione moiety as an ancillary ligand and a reaction site. Details of spectroscopy, electrochemistry, and ECL studies will be discussed in the presentation.

Poster Presentation : **ORGN.P-422**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Hierarchical Chirality Transfer of Peptide Foldamer

Jungwoo Hong, Jintaek Gong[1], 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*

Peptide foldamers synthesized from achiral amino acids usually forms only racemic helices, not having preference for a particular handness. Helical racemic property of achiral peptide foldamer can be broken by introducing chiral amino acid into peptide sequence, results in a stabilization of single helical configuration. Herein, we prepared series of chiral/achiral heptapeptide foldamers, consisted of four α- and three γ-amino acids. The ratio between two configurations was adjusted via variation of peptide residue and sequence. Co-assembly between chiral and achiral peptide foldamer yields foldecture—self-assembled architecture of foldamers—having the internal molecular packing structures with achiral peptide foldamers adopting single configuration; since only achiral peptide adopting helical structure capable of interacting with chiral peptide can participate in self-assembly process. This study enables hierarchical chirality transfer of peptide foldamer, essential for understanding peptide-peptide interaction under various self-assembly process, ultimately mimicking structural and functional features of natural proteins.

Poster Presentation : **ORGN.P-423**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Efficient and Safe Synthesis of Molecular Explosives via Flow Chemistry

Se Won Bae*, Sejin Lee[1]

Korea Institute of Industrial Technology, Korea
[1]Agency for Defense Development, Korea

The military continues to be interested in the development of Insensitive Munitions (IMs) while maintaining the effectiveness of the High Explosive (HE) composition. For example, 1-methyl-3,5-dinitro-1,2,4-triazole (MDNT) bridges the technical gap between Comp-B and IMX-104 through melt casting, while maintaining the performance and effectiveness of existing products. MDNT is currently being synthesized through Batch Chemistry (BC). However, synthesis through BC has shown problems in scalability, yield, and throughput, and generates large amounts of synthetic by-products, resulting in low economic efficiency and environmental problems. Accordingly, there is an urgent need for a more economical and environmentally friendly synthesis method that can replace BC.Flow Chemistry (FC) is emerging as a new way to replace BC because of its ease of scale-up, easy yield improvement, low synthetic by-products and the ability to perform the synthesis process very safely. The FC process is also attracting attention as a new alternative for developing new synthesis methods that were not possible in BC because of their excellent heat transfer capabilities.This study introduces the synthesis of molecular explosives using FC process. The FC process enabled the MDNT synthesis to be performed in a more environmentally friendly and cost-effective manner, increasing operator safety. Through efficient mixing process to increase the yield of the product, minimizing the waste solvent and synthetic by-products generated during the reaction process, the product was purified quickly and easily in a continuous process to increase the purity, and increased the safety of the operator.

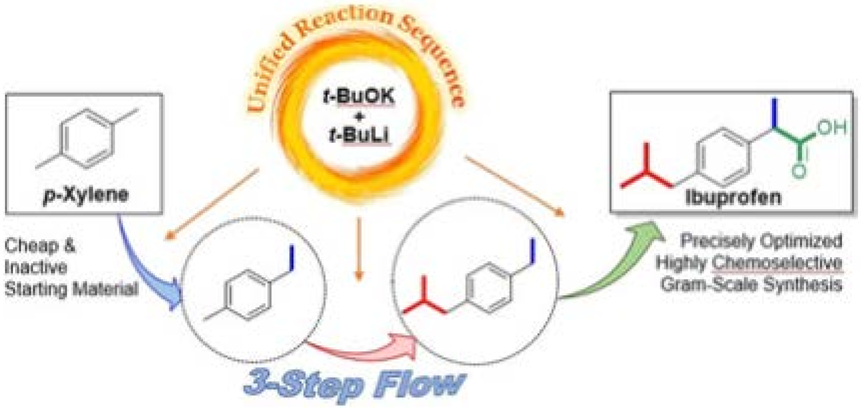
Poster Presentation : **ORGN.P-424**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

From p-Xylene to Ibuprofen in Flow: 3-Step Synthesis via Unified Sequence of Chemoselective C–H Metalations

Hyune-Jea Lee, Heejin Kim[1,*], Dong Pyo Kim[*]

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

Ibuprofen was prepared from an inactive and low-cost p-xylene by three-step flow synthesis through chemoselective metalations of benzyl positions using an in situ generated LICKOR-type superbase. The flow approach in the microreactor facilitated the comprehensive exploration of over 100 conditions in the first reaction step by varying concentrations, temperatures, solvents, and equivalents of reagents, enabling optimal conditions to be found with 95 % yield by significantly suppressing the competitive side reaction resulting in byproducts, followed by the second C−H metalation step in 95 % yield. Moreover, gram-scale synthesis of ibuprofen in the final step was achieved by biphasic flow reaction of solution-phase intermediate with gas phase carbon dioxide, isolating 2.3 g for 10 min of operation time.



Poster Presentation : **ORGN.P-425**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

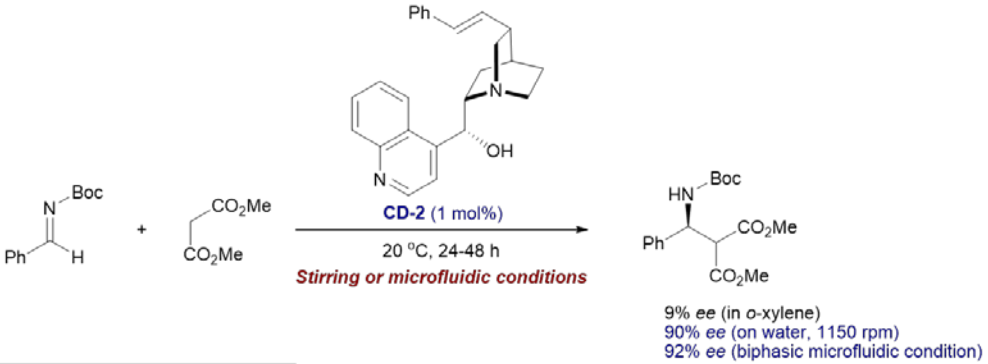
Chirality Amplification in Water Cages

Choong eui Song*, Si Joon Park, InSoo Hwang, Han Yong Bae[1], Jiyoon Jung

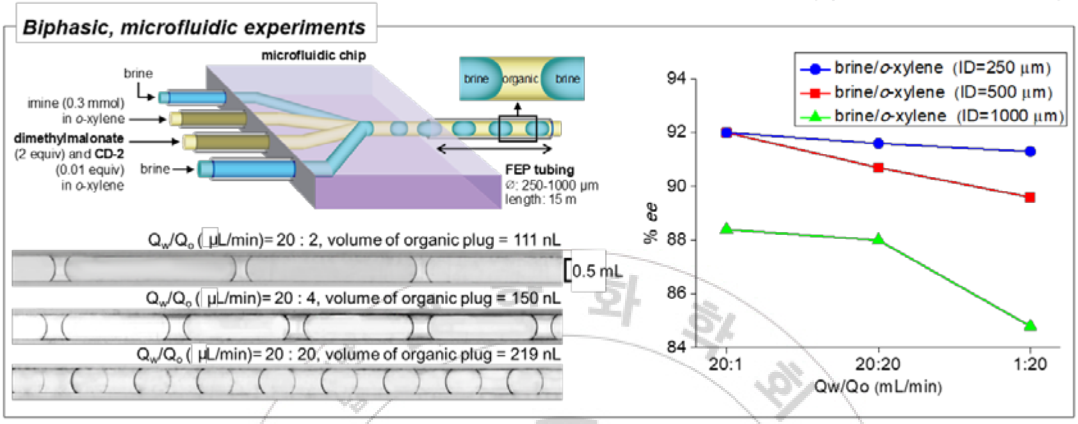
Department of Chemistry, Sungkyunkwan University, Korea

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

Homochirality is a fundamental component of molecular recognition in biological systems. Most theories for biological homochirality require a chiral amplification mechanism that acts to enhance a small initial asymmetry. We have found that water can induce the chirality amplification in a catalytic asymmetric reaction. Under on-water conditions, the enantioselectivity of a catalytic reaction can be significantly enhanced in the confined hydrophobic spaces of organic droplets surrounded by water. More significantly, this chirality amplification can be further increased by decreasing the droplet size. The droplet size effect on the enantioselectivity was quantified by using the biphasic microfluidic technique. Although in-depth mechanistic studies are still needed in order to fully understand the role of water, we can conclude that this water-induced chirality amplification can be attributed to the hydrophobically induced confinement effect. This remarkable observation could provide some inspiration for developing new strategies to enhance enantioselectivity and thus has the potential to open a new chapter in the field of asymmetric catalysis. In addition, our discovery that the enantioselectivity can be greatly amplified in the confined cavities of water cages could help unlock secrets of homochirality which is a fundamental component of molecular recognition in biological systems.



9% *ee* (in *o*-xylene)
90% *ee* (on water, 1150 rpm)
92% *ee* (biphasic microfluidic condition)



Poster Presentation : **ORGN.P-426**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Photochromic Reaction of Spiropyran-Anthracene Dyad

Hyeji Kim, Eun Ju Shin[1,*]

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

Spiropyran is the most widely studied photo-switchable compound. Upon irradiation of UV light to colorless and non-fluorescent spiropyran having two heterocyclic rings connected by a spiro carbon, spirocarbon-oxygen C-O bond is broken to form the highly conjugated zwitterionic merocyanine with a blue or violet color in solution. The merocyanine form returns to the original spirocarbon form thermally or on exposure to visible light. Anthracene is a typical polyaromatic compound which is strongly absorbing UV light and is easily forming pi-complex with other aromatic compound. Spectroscopic properties and photochromic reaction of Spiropyran-Anthracene dyad has been investigated by using ultraviolet-visible absorption and fluorescence spectroscopy.

Poster Presentation : **ORGN.P-427**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Photochromic Reaction of Spiropyran-sulfonate Containing Nitro Group

Seul Gi Hong, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

A spiropyran is a organic photochromic compound and is widely used in medical and technological areas. Photochromic, thermochromic, solvatochromic and electrochromic characteristics of spiropyrans make them especially important in the technology area. Most of their applications are based on their photochromic properties.Irradiation of colorless spiropyran in solution with UV light of wavelength 250–380 nm breaks C-O bonds of spiro ring and generates colored open-ring isomer merocyanine.Because of the apparent conjugated system formed after UV illumination, the extinction coefficient of the open-ring merocyanine form is significantly higher than the one of the closed-ring spiropyran form. Once the irradiation has stopped, the colored merocyanine in solution starts to discolour and to revert to its original colorless spiropyran. Depending on substituent in the aromatic system, the switching behaviour of the spiropyran derivatives can change in their switching velocity and photo-fatigue resistance. In this study, absorption and fluorescence spectra and reversible photochromic reaction of spiropyran-sulfonate containing nitro group has been investigated at various pH under UV or visible light on/off conditions.

Poster Presentation : **ORGN.P-428**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

pH Dependence on Spectroscopic Properties of Spiropyran-sulfonate Containing Methoxy Group

Gunhee Kim, Eun Ju Shin[*]

Department of Chemistry, Sunchon National University, Korea

Spiropyran-sulfonate is a sort of photoacid and is expected to carry out the pH-responsive light-controlled proton transfer reaction. Proton-transfer reactions are very important in biological processes and can be used to regulate chemical reactivity, biological functions, and material properties. Photoacid with stronger acidity in the excited state than in the ground state releases a proton upon light irradiation. Photoacid can be used to control protonations and deprotonations. Light as an external trigger can be applied with high precision of location, timing, and dosage. Reversible protonation and deprotonation reaction of photoacids can be used in molecular motors and acid-catalyzed reactions. We report here absorption and fluorescence spectral changes of sulfonate-functionalized spiropyran with methoxy substituent at various pH under UV or visible light on/off conditions.

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Poster Presentation : **ORGN.P-429**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Fe3+ Detection Based on Absorption Spectral Change of Rhodamine-thiophene

Bumhee Park, Eun Ju Shin[1,*]

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

The development of selective optical receptors for the detection of environmentally and biologically important metals has received much attention. Rhodamine exerts excellent photophysical properties such as long absorption and emission wavelengths, high molar extinction coefficient values and high emission quantum yield. Rhodamine is an optical colorimetric sensing probe suitable for the d-block metal cations.We report here a new rhodamine-based colorimetric/fluorometric sensing probe for the selective detection of metal cation. A rhodamine derivative with thiophene substituent has been prepared and characterized by IR, 1H NMR, and 13C NMR spectra. Its metal cation sensing ability has been investigated based on the absorption and fluorescence spectroscopic measurements. Especially, absorption of rhodamine derivative with thiophene substituent increase selectively with the presence of Fe3+ cation.

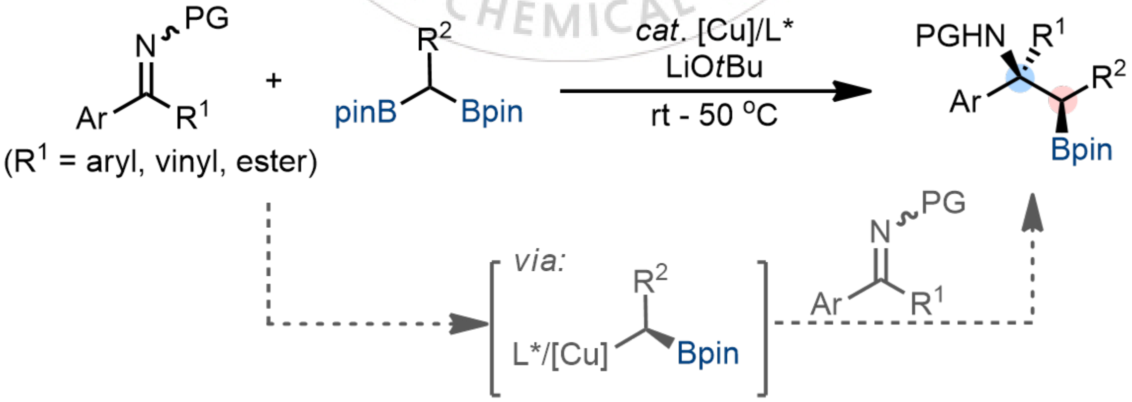
Poster Presentation : **ORGN.P-430**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Highly Diastereo- and Enantioselective Catalytic Addition of 1,1-Diborylalkanes to Ketimines Using Copper(I)-Catalysis

Jeongho Kim, Minkyeong Shin, Seung Hwan Cho*

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

Previously, we developed an efficient copper(I)-catalytic system for diastereo- and enantioselective 1,2-addition of 1,1-diborylalkanes to aldimines to afford chiral β-aminoboron compounds that can potentially be used to building blocks of synthetic chemistry. Therefore, We envisaged that the reaction of 1,1-diboryalkanes with ketimines would provide β-aminoboronate esters containing contiguous tetrasubstituted and trisubstituted stereocenters. However, this strategy is challenging because ketimines were knowns to be intrinsically less reactive than aldimines. Herein, we describe a broadly applicable copper catalytic conditions for the diastereo- and enantioselective 1,2-addition of 1,1-diborylalkanes to ketimines. Further transformations that convert the obtained β-aminoboronate esters to synthetically beneficial chiral building blocks are also demonstrated.



- Creation of adjacent chiral tertiary amines and secondary boronate esters
- Excellent diastereo- (up to >20:1) and enantioselectivity (up to 99% ee)
- Broad substrate scope

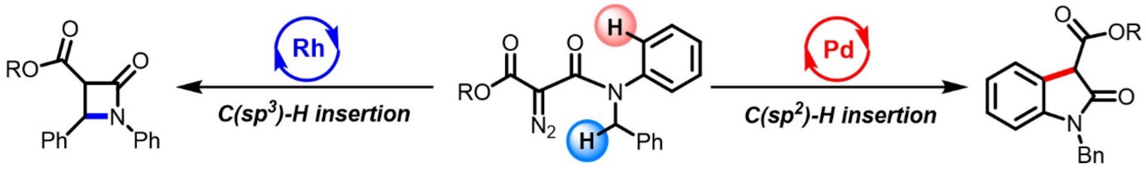
Poster Presentation : **ORGN.P-431**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Catalyst-Controlled Divergent C-H Bond Insertion of α-Diazoamides

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

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

Transition-metal catalyzed C-H bond functionalization has been widely developed wherein it could provide a convenient access to carbon-carbon bonds formation. Particularly, intramolecular C-H bond insertion of metal-carbenoids has been considered as one of the most efficient synthetic strategies for heterocycles. Despite considerable advances, selective insertion of metal carbenoids into the C(sp^3)-H and C(sp^2)-H bonds is not reported to date. Recently, we developed an asymmetric Rh(II)/Pd(0) relay catalysis for synthesis of chiral β-lactams through Rh(II)-catalyzed intramolecular enantioselective C(sp^3)-H insertion, followed by Pd(0)-catalyzed diastereoselective allylation. During our ongoing studies on Rh(II)/Pd(0) dual catalysis, we found that the catalyst-controlled divergent C(sp^3)-H / C(sp^2)-H insertion of α–diazoamides could be possible for synthesis of *N*-heterocycles, *i.e.*, the rhodium catalyst undergoes C(sp^3)-H insertion affording β-lactam derivatives, whereas the palladium catalyst undergoes C(sp^2)-H insertion affording indolin-2-one derivatives.



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Poster Presentation : **ORGN.P-432**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Enantioselective Radical Addition to Various Aldehydes Using Lewis Acid and Photoredox Catalyst

Jae Yeon Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Use of visible-light is regarded as attractive and advantageous method for development of selective and efficient synthetic methodology. To approach enantioselective visible-light induced photoredox catalysis, various synergistic catalysis have been developed recently. For example, transition-metal based photoredox catalyst coupled with chiral amine, Brønsted acid organocatalyst, and Lewis acid catalyst. In this research, we developed enantioselective radical addition to various aldehyde compounds in the presence of chiral Lewis acid catalyst and transition-metal based photoredox catalyst. Using this methodology, we synthesized highly optically active β-amino alcohol derivatives with good yields (up to 99%) and high enantioselectivities (up to 98% ee).

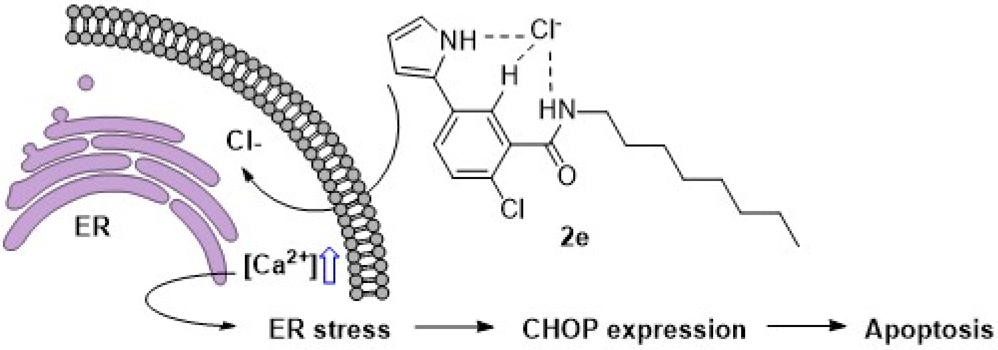
Poster Presentation : **ORGN.P-433**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthetic Anion Transporters as Endoplasmic Reticulum (ER) Stress Inducers

Jae Won Song, Min-sung Ko, Dong-gyu Cho*

Department of Chemistry, Inha University, Korea

Chloride ion transporters (**2a–2h**) were synthesized based on the binding motifs of prodigiosin. Transporter **2e** clearly displays Cl^- ion transportation activity across both model and live cell membranes. Furthermore, **2e** can disrupt Ca^{2+} homeostasis and increase the intracellular concentration of Ca^{2+} in DLD-1 cell. This disruption can lead to Caspase-dependent apoptosis supported by CHOP expression (a marker of ER stress) and the appearance of the cleaved forms of Caspase 3 and PARP.



Poster Presentation : **ORGN.P-434**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Photodynamic Therapy of Iridium complexes by Lysomal Protein Oxidation

Mingyu Park, Tae-Hyuk Kwon[1,*], Sungjin Park[2], Taiho Park[3]

Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Eco-Friendly Energy Engineering, Ulsan National Institute of Science and Technology, Korea*
[2]*Chemical Engineering, Pohang University of Science and Technology, Korea*
[3]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

Efficacy of lysosome targeting iridium photodynamic therapy agent was studied followed by mass spectrometric proteome analysis. Iridium complexes with lysosome targeting morpholine moiety showed high biocompatibility under dark condition and effective cancer cell suppression via reactive oxygen species generation. Photophysical properties were analyzed and in vitro cell tests were done including MTT assay. Also, target motions of iridium series were investigated by confocal microscopy.

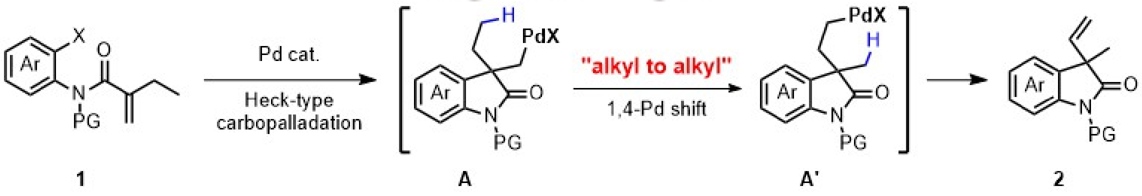
Poster Presentation : **ORGN.P-435**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

An Efficient Synthesis of Quaternary Vinylated Oxindoles by Alkyl to Alkyl Palladium Migration

Da Sol Chung, Jiwon Hwang, Sang-gi Lee*

Department of Chemistry and Nanoscience (BK 21 PLUS), Ewha Womans University, Korea

Transition metal-catalyzed C-H bond functionalization is widely developed due to its powerful and atom-economic advantage. To enable through-space interaction of a metal center with a neighboring C-H bond, metal migration strategy, including a C-H activation for forming a five membered palladacycle intermediate, has been frequently utilized. However, most reported 1,4-Pd migrations were limited to alkyl C(sp^3)-Pd to aryl C(sp^2)-Pd or aryl C(sp^2)-Pd to aryl C(sp^2)-Pd migrations. No research on alkyl C(sp^3)-Pd to alkyl C(sp^3)-Pd migration was reported. During our recent study on regiodivergent cyclopropanation of σ-alkylPd(II)-intermediate **A** generated by Heck-type carbopalladation, unprecedented alkyl C(sp^3)-Pd to alkyl C(sp^3)-Pd migration was observed, from intermediate **A** to **A'**, and it underwent β-hydride elimination to afford the quaternary vinylated oxindoles **2**. To the best of our knowledge, this is the first example of an alkyl to alkyl 1,4-Pd migration.



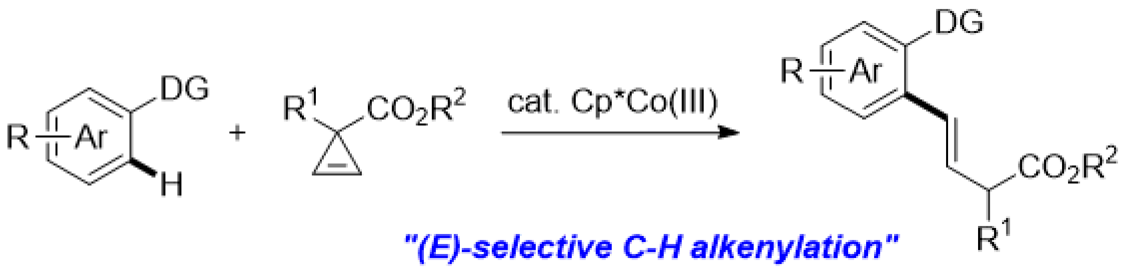
Poster Presentation : **ORGN.P-436**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

(E)-Selective C-H Alkenylation of (Hetero)arenes under Cobalt(III) Catalysis

Suh Young Choi, Juhyun Kim*

Department of Chemistry, Gyeongsang National University, Korea

From the past decades, tremendous efforts have been directed towards the development of transition metal-catalyzed C-H bond activation reactions, which allows the direct functionalization of generally inert C-H bonds. Among various functional groups, alkenyl group has been extensively applied to C-H bond activation strategy while using terminal/internal alkynes and linear alkenes as surrogates for the alkenyl moiety. Despite their remarkable importance and thus achieved considerable advances, C-H alkenylation reactions still suffer from two major issues; one is that the most of the previous reports on C-H alkenylaton relied on only terminal/linear alkynes and alkenes as coupling partners and another is controlling E/Z selectivity with broader scope of substrates. In this study, we present cobalt(III)-catalyzed (E)-selective C-H alkenylation reaction of (hetero)arenes without any double-alkenylation product. The present catalytic system will be expected to set the stage for step- and atom-economic C-H bond activation of arenes and heteroarenes, thereby providing versatile synthetic route to a variety of alkenyl-substituted (hetero)arenes.



"(E)-selective C-H alkenylation"

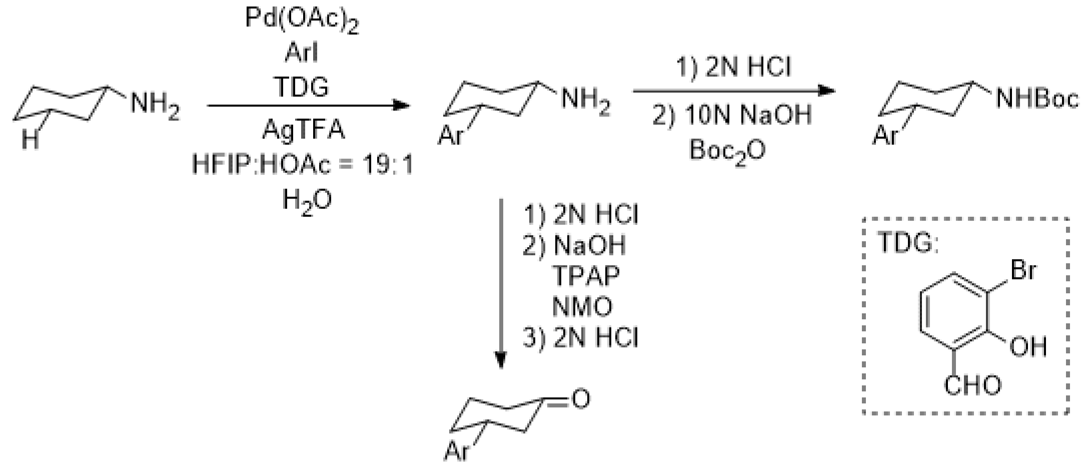
Poster Presentation : **ORGN.P-437**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

β-Functionalization of Ketone via Pd-Catalyzed γ-C(sp3) Arylation of Cyclohexylamine with a Transient Directing Group

Hahyoun Park, Yunyeong Gwon, Byunghyuck Jung[1,*]

School of Undergraduate Studies, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*School of Basic Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Research of C-H activation has been conducted in worldwide because of its applicability that C-H bond can be exchanged with C-X bond (X= C, O, N, etc.). To activate specific C-H bond, transient directing group is needed for high regioselectivity and efficiency. Therefore, we found the reaction condition and efficient transient directing group to activate γ-C(sp3)-H bond of cyclohexylamine. As a result, 3-bromosalicylaldehyde is the most effective transient directing group in promoting C-H arylation. This reaction progressed with substituted aryl iodides regardless of electronic properties and position of substituent. Both of Electron-rich and electron-deficient aryl iodides afforded the desired products with good yield. In addition, aryl iodides bearing substitutions at the ortho, meta and para position are also well tolerated. Furthermore, C-H arylation proceeded with aliphatic amine, cyclopentyl amine and cycloheptyl amine.To demonstrate the utility of this reaction, further research is being carried out to obtain desired ketone product from substituted amine. Ketone is an important precursor in organic chemistry. Herein we have synthesized β- substituted ketone from γ-substituted amine compound. Substituted amine compound oxidized to imine using TPAP and NMO. Then imine compound converted to ketone after adding hydrochloric acid solution. To synthesize β- substituted ketone, 1,4-addition of enone using Gilman reagents is usually used. However, when Gilman reagents have electrophilic substituent such as carbonyl group, desirable ketone cannot be obtained. Through this reaction, diverse arylated ketone can be synthesized with any substituent regardless of its electronic properties.


Pd(OAc)2
ArI
TDG
AgTFA
HFIP:HOAc = 19:1
H2O
NH2
H
NH2
Ar
1) 2N HCl
2) 10N NaOH
Boc2O
NHBoc
Ar
1) 2N HCl
2) NaOH
TPAP
NMO
3) 2N HCl
O
Ar
TDG:
Br
OH
CHO

Poster Presentation : **ORGN.P-438**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

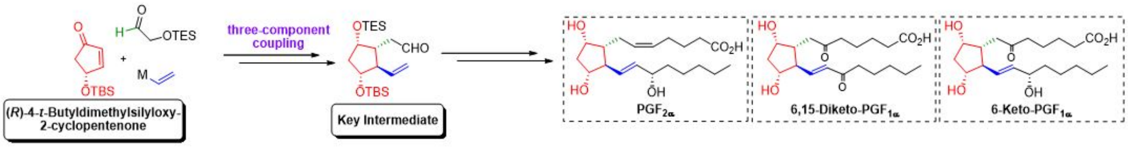
Total Synthesis of PGF2α and 6,15-Diketo-PGF1α and Formal Synthesis of 6-Keto-PGF1α via Three-Component Coupling

Taehyeong Kim, **Do Hyun Ryu**[*]

Department of Chemistry, Sungkyunkwan University, Korea

Prostaglandins (PGs) are a group of naturally occurring lipid compounds. They exist in animals and human-beings and mediate various physiological functions[1]. PGs contain 20 carbon atoms including a five-membered carbon ring and have several types of analogues which vary in carbon ring and upper and lower side chain structures. Due to their wide array of bioactivities[2], PGs have attracted considerable attention from synthetic chemists and numerous synthetic explorations have been implemented over several decades[3]. Our research group interested in synthesis of PGF2α which is known for its luteolytic effect (degradation of the corpus luteum) in cattle[4] and prostacyclin (PGI2) which has excellent ability to inhibit platelet aggregation and vasodilation[2]. One of the PGF2α analogues, latanoprost (Xalatan) is using for treatment of glaucoma and quickly became a "blockbuster" drug for Pfizer, with sales of $1.75 billion in 2010[5]. Because PGI2 is unstable in aqueous conditions and rapidly decomposed to its metabolites; for instance, 6,15-diketo-PGF1α and 6-keto-PGF1α are known metabolites of prostacyclin[6]. Compared with PGF2α, synthetic studies on PGI2 and its stable metabolites, 6,15-diketo-PGF1α and 6-keto-PGF1α have rarely been reported[3(b)]. To the best of our knowledge, there is no synthetic example for 6,15-diketo-PGF1α and only one example of total synthesis of 6-keto-PGF1α from simple starting material was reported[7] in spite of their many analytical studies[6(c),8].Considering the same core structures of them, we envisioned that three target compounds would be synthesized from common intermediate because appropriate functional groups can be easily introduced for the installation of both side chains. Herein, we reported an efficient synthetic route to PGF2α, 6,15-diketo-PGF1α and 6-keto-PGF1α with high levels of stereoselectivity from a common synthetic intermediate.References :1.(a) Gibson, K. H. Chem. Soc. Rev. 1977, 6, 489-510; (b) Curtis-Prior, P. B. Prostaglandins: Biology and Chemistry of Prostaglandins and Related Eicosanoids, Churchill Livingstone, New York, 1988; (c) Marks, F.; Fürstenberger, G. Prostaglandins, Leukotrienes and other Eicosanoids, Wiley-VCH, Verlag, New York, 1999 and references therein; (d) Dams, I.; Wasyluk, J.; Prost, M.; Kutner, A. Prostaglandins Other Lipid Mediators 2013, 104-

105, 109-121.2.Collins, P. W.; Djuric, S. W. Chem. Rev. 1993, 93, 1533-1564.3.(a) Das, S.; Chandrasekhar, S.; Yadav, J. S.; Grée, R. Chem. Rev. 2007, 107, 3286-3337; (b) Peng, H.; Chen, F.-E. Org. Biomol. Chem. 2017, 15, 6281-6301.4.(a) Lauderdale, J. W. J. Anim. Sci. 2008, 87, 801. (b) Rowson, L. E. A.; Tervit, R.; Brand, A. J. Reprod. Fertil. 1972, 29, 145.5.Full-year results for 2010 were reported by pfizer: http://www.pfizer.com/Files/investors/presentations/q4performance_020111.pdf6.(a) Cho, M. J.; Allen, M. A. Prostaglandins 1978, 15, 943-954; (b) Armstrong, J. M.; Thirsk, G.; Salmon, J. A. Hypertension 1979, 1, 309-315; (c) Etingin, O. R.; Weksler, B. B.; Hajjar, D. P. J. Lipid. Res. 1986, 27, 530-536.7.Tanaka, T.; Hazato, A.; Bannai, K.; Okamura, N.; Sugiura, S.; Manabe, K.; Toru, T.; Kurozumi, S.; Suzuki, M.; Kawagishi, T.; Noyori, R. Tetrahedron 1987, 43, 813-824.8.(a) Falardeau, P.; Oates, J. A.; Brash, A. R. Anal. Biochem. 1981, 115, 359. (c) Rosenkranz, B.; Fischer, C.; Weimer, K. E.; Froelich, J. C. J. Biol. Chem. 1980, 255, 10194.



Poster Presentation : **ORGN.P-439**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Asymmetric Methallylation and Allylation Reactions with Silane Compounds Catalyzed by a Chiral Lewis Acid

Taehyeong Kim, Hye Min Jeong[1], Do Hyun Ryu[*]

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

The asymmetric methallylation and allylation of aldehydes are one of the carbon–carbon bond-forming reactions in chemical synthesis and have been regarded as a testing ground for new asymmetric methodology. Enantiomerically pure homoallylic alcohols are common synthetic intermediates. The enantioselective methallylation of aldehydes is also important asymmetric transformations in organic synthesis, but rather less developed. Homoallylic alcohols are typically generated by allylmetal-aldehyde addition reactions. A novel strategy has been developed for an enantioselective methallylation and allylation reaction of aromatic and aliphatic aldehydes with silane compounds catalyzed by a chiral Lewis acid. Silane compounds possess high thermal stability, nontoxicity, and rather low sensitivity to moisture and oxygen. In the end, the reaction provides homoallylic alcohols in good yields and with high enantioselectivity. This reaction shows promising utility in various other challenging chemical reactions and conspicuous biological activity.[References]Kaib, P. S. J.; Schreyer, L.; Lee, S.; Properzi, R.; List, B. *Angew. Chem. Int. Ed.* 2016, *55* , 13200-13203.Mahlau, M.; Garcia-Garcia, P.; List, B. *Chem. Eur. J.* 2012, *18* , 16283-16287Konishi, S.; Hanawa, H.; Maruoka, K. *Tetrahedron : Asymmetry*., 2003, *14* , 1603-1605

Poster Presentation : **ORGN.P-440**

Organic Chemistry

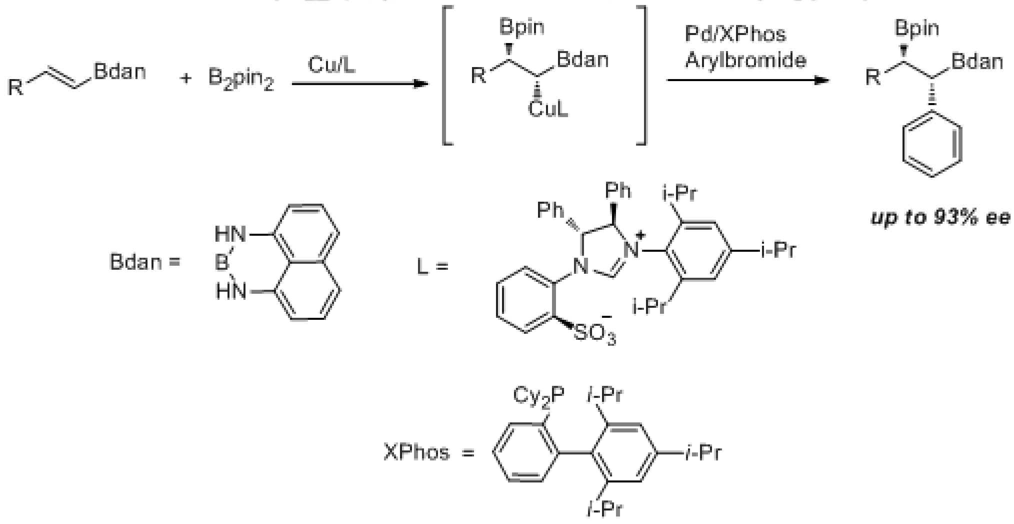
Exhibition Hall 1, FRI 11:00~12:30

Pd/Cu-Catalylzed Diastero- and Enantioselective Arylboration of Borylalkenes

Hyesu Lee, **Lee Soyeon**[1], **Jaesook Yun**[*]

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

We have developed the Pd/Cu-catalyzed diastereo- and enantioselective arylboration of borylalkenes using B_2pin_2 as a boron source and arylbromide as cross-coupling partner. Combination of NHC(N-heterocyclic carbene)-copper catalyst and palladium-XPhos catalyst afforded the corresponding products containing two different boryl groups in an *anti*-configuration with good enantioselectivities up to 93% ee. Selective transformations of Bpin to alcohol and trifluoroborate salt by reactivity difference between two boryl moieties demonstrate the synthetic utility of the product.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Poster Presentation : **ORGN.P-441**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Characterization of Ultraviolet curable coating agent using urethane acrylate

Eun Ji Park

Advanced material research division, Korea Institute of Footwear & Leather Technology, Korea

With the recent increase in national income, the outdoor market is greatly developing. In addition, high-quality design and pattern implementation technology and eco-friendly coating technology are needed due to the high quality and eco-friendly problems of leisure, sports and living textile materials. In addition, the clothing pattern is a method of coating using a thermosetting coating agent containing an organic solvent. This method generates a large amount of VOCs in the coating process and reduces productivity. In order to apply the three-dimensional precision pattern of fibers, in this study, we synthesized and characterized the solvent-free type UV curable composite resin. The coatings synthesized through this study are expected to be used not only in the textile industry but also in various coating industries such as construction and automobiles.AcknowledgementThis work was supported by the Industrial Technology Innovation Program (20000372) funded By the Ministry of Trade, industry & Energy(MI, Korea)

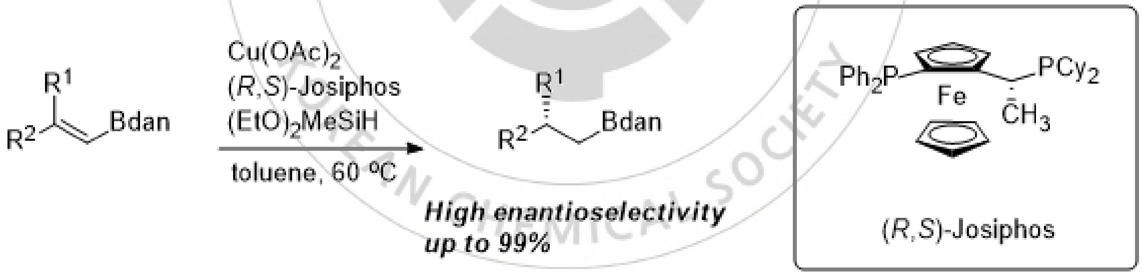
Poster Presentation : **ORGN.P-442**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

β-Chiral Organoboron Compounds through Copper-Catalyzed Enantioselective Reduction

<u>Yeji Park</u>, Jaesook Yun[*]

Department of Chemistry, Sungkyunkwan University, Korea

Highly enantioselective reduction of *β,β*-disubstituted alkenyl boramide compounds employing copper catalyst and hydrosilanes was investigated. In the presence of a copper(Ⅱ) catalyst with chiral Josiphos ligand, a range of alkenyl boramide compounds with primary or secondary alkyl, silyl and aryl substituent(R^2) produced chiral disubstituted boramide compounds in good yield with high enantioselectivity up to 99% ee.



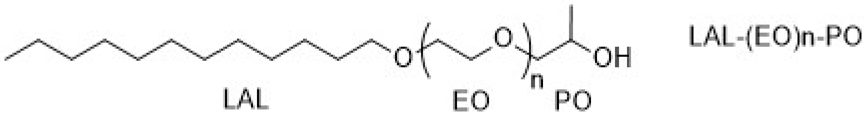
Poster Presentation : **ORGN.P-443**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Purification and characterization of surfactant intermediate LAL-(EO)n-PO derivatized from lauryl alcohol (LAL) with ethylene oxide and propylene oxide

Md. Maniruzzaman Manir, Surk-Sik Moon*, Byeong Jo Kim[1], Hyon Pil Yu[2], Seok-Hyeon Kim[3]

Department of Chemistry, Kongju National University, Korea
[1]*R&D Center, AK CHEMTECH, Korea*
[2]*계면연구팀, AKCHEMTECH, Korea*
[3]*Surfactant R&D team, AKCHEMTECH, Korea*

The reaction mixture prepared from the reaction of lauryl alcohol with ethylene oxide was fractionated by silica gel column chromatography (Silica MPLC) to provide each ethylene oxide and propylene oxide-reacted lauryl alcohol. Each component was unambiguously characterized by using spectroscopic methods including 1D and 2D NMR (COSY, HSQC, and HMBC) spectroscopy. The average number of ethylene oxide (EO) and propylene oxide (PO) unit in the mother mixture was estimated by NMR analysis of the mother adduct mixture.



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-444**

Organic Chemistry

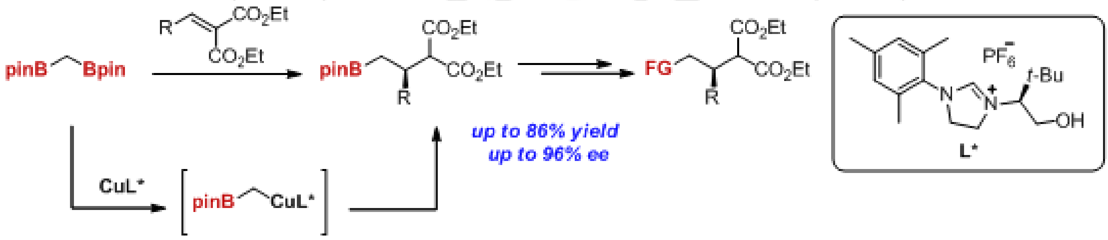
Exhibition Hall 1, FRI 11:00~12:30

Copper-Catalyzed Enantioselective Conjugate Addition of 1,1-Diborylmethane to α,β-Unsaturated Diesters

Won Jun Jang, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Catalytic asymmetric conjugate addition of borylalkyl copper complex formed in situ by 1,1-diborylmethane to α,β-unsaturated diesters has been developed. This reaction provides an efficient synthetic method of β-chiral alkylboron diesters in good yields with high enantioselectivities. The resulting enantioenriched organoboron compounds were stereospecifically transformed to various organic compounds with retention of the original enantioselectivities.



Poster Presentation : **ORGN.P-445**

Organic Chemistry

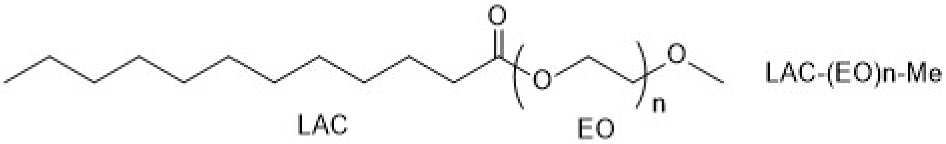
Exhibition Hall 1, FRI 11:00~12:30

Characterization of surfactant intermediate LAC-(EO)n-Me prepared from the reaction of lauric acid (LAC) with ethylene oxide followed by methylation.

Md. Maniruzzaman Manir, Surk-Sik Moon*, Byeong Jo Kim[1], Kiho Park[2], Jihye Bae[2]

Department of Chemistry, Kongju National University, Korea
[1]*R&D Center, AK CHEMTECH, Korea*
[2]*AKCHEMTECH, Korea*

Surfactant intermediates prepared from lauric acid with ethylene oxide followed by methylation were purified by silica gel column chromatography (Silica MPLC) to provide each lauric acid-ethylene oxide adduct. Each component was fully characterized via spectroscopic methods including 1D and 2D NMR (COSY, HSQC, and HMBC) spectroscopy, revealing the number of ethylene unit. From the NMR information of each adduct, the average number of ethylene oxide unit in the mother mixture was estimated by NMR analysis of the mixture.



Poster Presentation : **ORGN.P-446**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Synthesis structures and spectroscopic properties of mono and dimeric BODIPYs

Galam Jung, Se Won Bae[1,*]

Chemistry, Sungkyunkwan University, Korea / Green Chemistry and Materials Group, Korea Institute of Industrial Technology, Korea
[1]*Green Chemistry and Materials Group, Korea Institute of Industrial Technology, Korea*

The boron dipyrromethenes (BODIPYs) have attracted great attention in recent decades with high molar extinction coefficients, fluorescent quantum yields, negligible triplet state formation, narrow emission bandwidths with high peak intensities, excellent thermal and photochemical stabilities. The electronic and photophysical properties of BODIPYs can be fine-tuned for different applications by the structural modification of the boron-dipyrrin core or by making their dimers and oligomers. Reports on covalently linked BODIPY dimers are on the rise but still there is a need to study the photophysical properties of mono and bridged BODIPY dimers. In this work, we focus our work on the meso-meso linked dimeric BODIPYs and mono BODIPYs with different alkyl substituents. In this contribution, we present the structure of BODIPYS, NMR, MALDI-MS, photophysical properties.

Poster Presentation : **ORGN.P-447**

Organic Chemistry

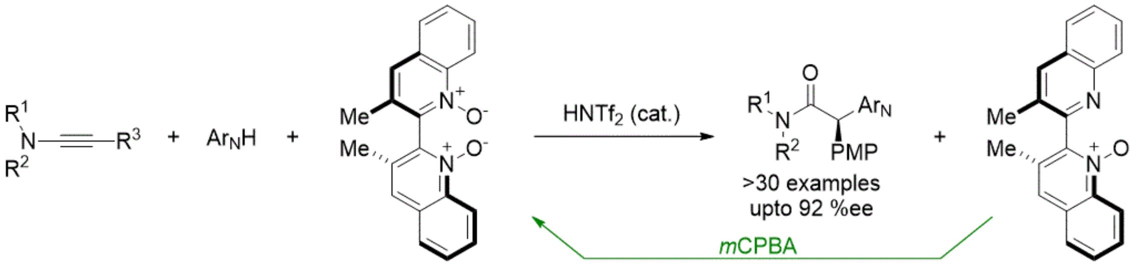
Exhibition Hall 1, FRI 11:00~12:30

Enantioselective Oxygenative Arylation of Ynamides Employing Chiral *N*-Oxides

Tae-Woong Um, Girim Lee, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Synthesis of α-aryl carbonyl compounds is important because an array of natural products and pharmaceutically relevant molecules contain this moiety.[1] The introduction of aryl groups at the α-position of carbonyl compounds was initially addressed in the Pd-catalyzed cross-coupling of enolate species with aryl halides.[2] However, strong base involved limited their applications in the synthesis of tertiary α-arylated carbonyl compounds, due to a facile racemization of the product.[3]A potential solution to this synthetic problem has recently emerged, employing Brønsted acid-catalyzed oxygenative arylation of ynamides.[4] These processes occur under mildly acidic conditions, and thus the racemization can be kept to a minimum. We introduce an external oxidant. Herein, we report a reagent-controlled enantioselective oxidation reaction, using a chiral *N,N'*-dioxide. In this external oxidant approach, unmodified nucleophilic arenes could be employed and the product is now free of trace groups from the oxidant, thereby avoiding two unnecessary steps. Furthermore, the byproduct of the oxidation (mono-*N*-oxide) could be recycled at the end in an efficient manner. Various nucleophilic arenes, including indoles, phenols, and pyrroles, participate in the oxygenative alkylation, and enantioselectivity upto 92%ee was realized.Reference1. Bellina, F.; Rossi, R. *Chem*. *Rev*. **2010**, *110*, 1082-1146. (b) Johansson, C. C. C.; Colacot, T. J. *Angew*. *Chem*. *Int*. *Ed*. **2010**, *49*, 676-707.2. Hamann, B. C.; Hartwig, J. F. *J*. *Am*. *Chem*. *Soc*. **1997**, *119*, 12382-12383.3. Chae, J.; Yun, J.; Buchwald, S. L. *Org*. *Lett*. **2004**, *6*, 4809-4812.4. (a) Kaldre, D.; Maryasin, B.; Kaiser, D.; Gajsek, O.; González, L.; Maulide, N., *Angew*. *Chem*. *Int*. *Ed*. **2017**, *56*, 2212-2215. (b) Kaldre, D.; Maulide, N. *Science*, **2018**, *361*, 664-667.



>30 examples
upto 92 %ee

Poster Presentation : **ORGN.P-448**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

Silica-gel supported One-pot Synthesis of 2-Amido benzo[b]thiophenes

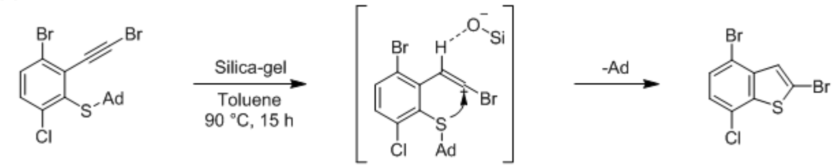
Solbin Kim, Hyun Suk Yeom[1,*]

Chemistry, Hanyang University, Korea

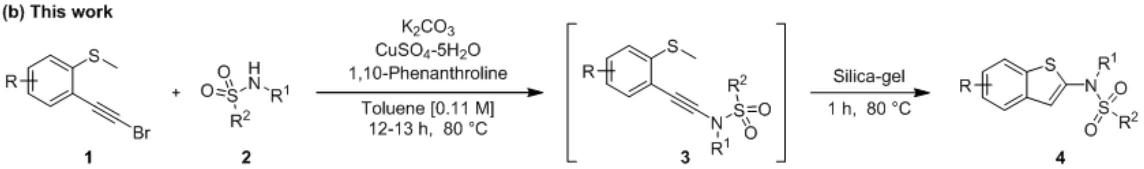
[1]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

Benzo[b]thiophenes are widely applied scaffolds in pharmaceutical and materials sciences. Thus, the synthesis of benzo[b]thiophenes has attracted great attention over the past few decades; a number of synthetic routes for 2-substituted or 2,3-disubstituted benzo[b]thiophenes through intra- and intermolecular reactions have been reported. However, in case of synthesis of 2-amido benzo[b]thiophenes, few cases using halogen reagents (I2, NBS, and NCS) and transition-metal catalysts (Au and Rh) have been disclosed so far.Recently, Toyota group reported the silica-gel assisted synthesis of 2-bromo benzo[b]thiophenes from the corresponding 2-(bromoethynyl)adamantylsulfide. Based on the preliminary results, we have tried the synthesis of 2-amido benzo[b]thiophenes from (o-thioanisole) substituted ynamides and desired products were obtained in high yields. Under careful optimization, one-pot reaction of ynamide coupling and cyclization reaction could be achieved by use of silica-gel as the promoter. This practical one-pot reaction affords an eco-friendly and economical synthetic route to 2-amido benzo[b]thiophenes with high yields in mild condition. This method is not relying on expensive transition-metal catalysts, no poisonous halogenated reagent, no additional purification of ynamide intermediates, and no extraction procedure of reaction mixture, which shows a power of this chemistry.

(a) Previous work



(b) This work



124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-449**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Pd-Catalyzed Three-Component-Coupling Reactions of Heteroarenes and Strained Alkenes

Eunmin Kim, Si Yeon Jung, Jung Min Joo*

Department of Chemistry, Pusan National University, Korea

Diheteroaryl ethylenes have found a broad spectrum of applications in drug discovery and materials science. Herein, we report a three-component-coupling reaction of haloheteroarenes, strained alkenes and another group of heteroarenes by palladium catalysis. Subsequently, diheteroaryl ethylenes having different heteroarenes were synthesized by retro-Diels-Alder (*r*DA) reactions. Although many methods for the synthesis of (*E*)-diheteroaryl alkenes have been reported, methods synthesizing the (*Z*)-forms are rare. Our method will be useful for the preparation of both (*Z*)-diheteroaryl alkenes as well as the (*E*)-counterparts.

Poster Presentation : **ORGN.P-450**

Organic Chemistry

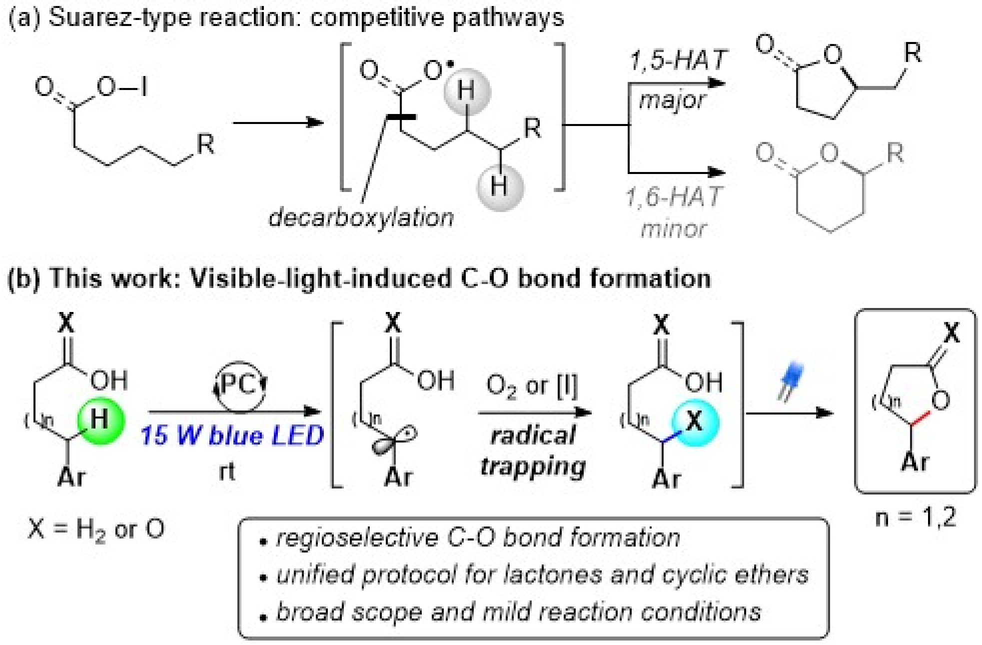
Exhibition Hall 1, FRI 11:00~12:30

Visible-Light Induced C-O Bond Formation for Construction of Cyclic Ethers and Lactones

Honggu Im, **Sungwoo Hong**[*]

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

Intramolecular benzylic C−O bond formation was developed using 2,4,6-triphenylpyrylium tetrafluoroborate (TPT), which allows construction of cyclic ethers and lactones. The reaction is supposed to proceed through the single-electron oxidation of the phenyl group, followed by the formation of a benzylic radical, thus preventing a competing 1,5-hydrogen abstraction pathway. Detailed mechanistic studies suggest that molecular oxygen is used to trap the radical intermediate to form benzyl alcohol, which undergoes cyclization. This new approach serves as a powerful platform by providing efficient access to valuable 5- and 6-membered cyclic ethers and lactones with a unified protocol.ReferenceIm, H.; Kang, D.; Choi S.; Shin S.; Hong, S.[*] *Org*. *Lett*. **2018**, *20*, 7437.



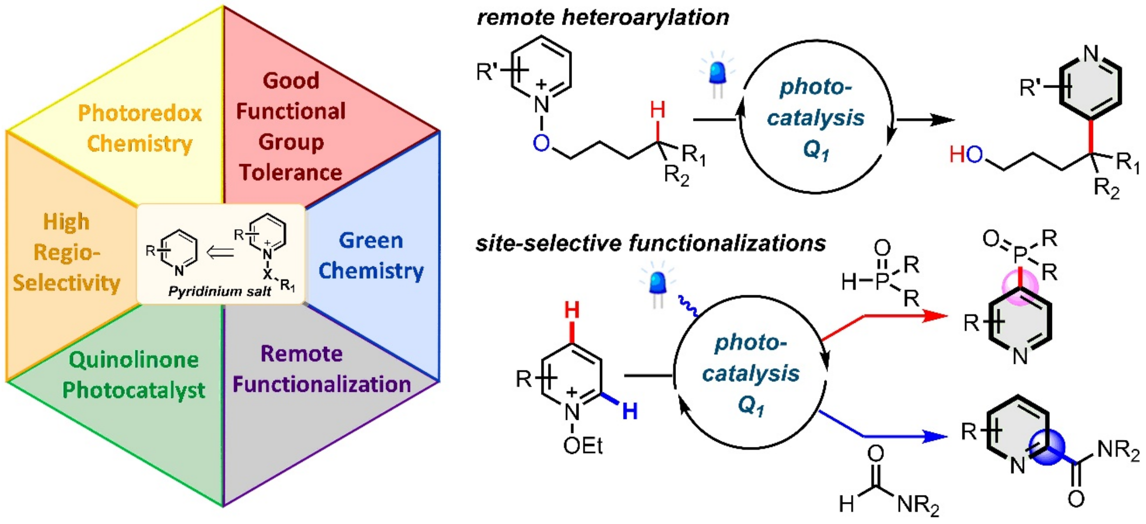
Poster Presentation : **ORGN.P-451**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Remote and Site-Selective Functionalization of Pyridinium Salts via Quinolinone Photocatalysis

Inwon Kim, Sungwoo Hong[*]

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

Visible-light-induced site-selective heteroarylation of remote C(sp^3)–H bonds has been accomplished through the design of N-alkoxyheteroarenium salts as both alkoxy radical sources and heteroaryl group sources. The alkoxy radical can be generated through the single electron reduction of N-alkoxypyridinium derivatives by a photoexcited quinolinone catalyst ($\mathbf{Q_1}^*$). Subsequent radical translocation (1,5-HAT) of the O-centered radical forms a C-centered radical intermediate, which undergoes addition to the pyridinium substrate to achieve remote C(sp^3)–H heteroarylation. This strategy provides a powerful platform for remote C(sp^3)–H heteroarylation in a controllable and selective manner for the synthesis of a broad range of 4-heteroaryl alcohol products which have quaternary, tertiary, and secondary carbon centers. Also we developed a new approach to site-divergent pyridine functionalization that offers considerable advantages in both simplicity and efficiency. The site-selectivity can be switched from C2 to C4 by changing the radical coupling sources. Under standard reaction conditions, phosphinoyl radicals give access to C4 products, while carbamoyl radicals selectively give C2 products. These current methods are well suited for late-stage functionalization of complex bioactive molecules. References[1] I. Kim, G. Kang, K. Lee, B. Park, D. Kang, H. Jung, Y.-T. He, M.-H. Baik, S. Hong, *J. Am. Chem. Soc.* **2019,** *141*, 9239.[2] I. Kim, B. Park, G. Kang, J. Kim, H. Jung, H. Lee, M.-H. Baik, S. Hong, *Angew. Chem. Int. Ed.* **2018,** *57*, 15517.[3] I. Kim, M. Min, D. Kang, K. Kim, S. Hong, *Org. Lett.* **2017,** *19*, 1394.[4] Y. Kim, K. Lee, G. R. Mathi, I. Kim, S. Hong, *Green Chem.* **2019,** *21*, 2082.[5] F.-S. He, S. Ye, J. Wu, *ACS Catal.* **2019,** *9*, 8943.


Photoredox Chemistry
Good Functional Group Tolerance
Green Chemistry
Remote Functionalization
Quinolinone Photocatalyst
High Regio-Selectivity
Pyridinium salt
remote heteroarylation
photo-catalysis Q_1
site-selective functionalizations
photo-catalysis Q_1
OEt
HO

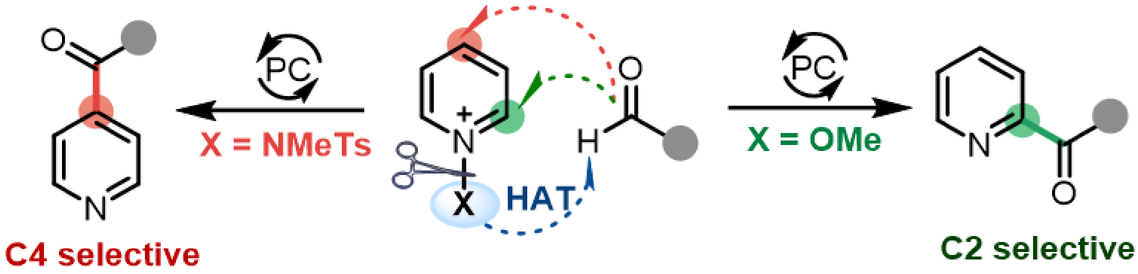
Poster Presentation : **ORGN.P-452**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

Site-Selective C–H Acylation of Pyridine Scaffolds by Photoredox Catalysis

Sungwoo Jung, Sungwoo Hong*

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

Despite several recent advances about acylation of pyridine moieties, existing methods remain limited mainly to the introduction of the acyl group to the C2-position of the pyridine scaffold, and the C4-acylation of pyridines has yet to be reported with meaningful selectivity. Herein, we developed a new strategy for visible-light-promoted site-selective C–H acylation of pyridinium salts by employing *N*-methoxy- or *N*-aminopyridinium salts, providing a powerful synthetic tool for accessing highly valuable C2- and C4-acylated pyridines. The methoxy or amidyl radicals photocatalytically generated from the pyridinium salts can abstract the hydrogen atom from readily available aldehydes to form acyl radicals, which can engage in addition to pyridinium derivatives. Remarkably, the use of *N*-methoxypyridinium salts preferentially gives the C2-acylated pyridines, and the site selectivity can be changed from C2- to C4-position by using *N*-aminopyridinium salts. The utility of this method was further demonstrated by the late-stage modification of complex biorelevant molecules and by application of acyl radicals to photoredox-catalyzed radical cascade reactions.



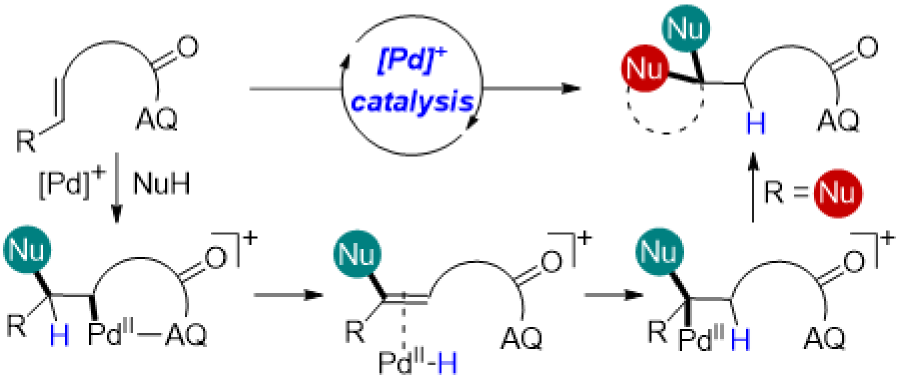
Poster Presentation : **ORGN.P-453**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

1,1-Difunctionalization of Unactivated Alkenes through Cationic Palladium Catalysis

Jinwon Jeon, Sungwoo Hong*

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

1,2-Difunctionalization of alkenes has been intensively developed utilizing alkene polarization by π-Lewis acid activation of transition metals. In opposition to outstanding advances in 1,2-vicinal difunctionalization, a similar example for 1,1-geminal difunctionalization of unactivated alkenes, while highly appealing, remains elusive.Herein, we describe a palladium(II)-catalyzed 1,1-difunctionalization of unactivated terminal and internal alkenes using cationic palladium(II) catalysis. After initial addition of a nucleophile to the alkene, the in situ generated stable palladacycle intermediate can be broken by a cationic palladium(II) catalyst to facilitate regioselective β-hydride elimination. Site-selective oxidative 1,1-difunctionalization is achieved with two nucleophilic components, even with challenging internal cyclic and acyclic alkene substrates. Various electron-rich arene nucleophiles, such as indoles and anilines, add to alkene moiety of 3-, or 4-alkenamides to give γ,γ- or δ,δ-di-functionalized products in fully intermolecular systems. Furthermore, employing intramolecular hydroxyl, carboxyl nucleophiles with external carbon nucleophiles, this method is further extended to unsymmetric difunctionalization, offering a powerful platform for making (oxo) quaternary carbon centers. Detailed computational results point to a reaction mechanism in which the cationic palladium(II) catalysis plays an important role in facilitating the key β-H elimination and migratory insertion steps.



- *site-selective 1,1-difunctionalization*
- *regioselective β-H-elimination*
- *C–H, O–H nucleophile*
- *quaternary carbon center*

Poster Presentation : **ORGN.P-454**

Organic Chemistry

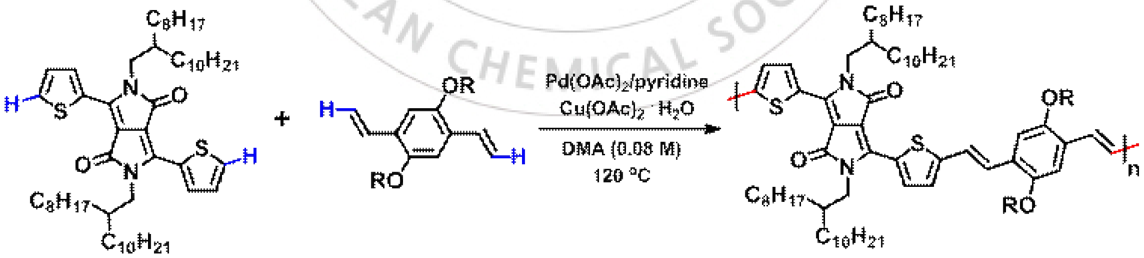
Exhibition Hall 1, FRI 11:00~12:30

Synthesis and Characterization of DPP-Based Conjugated Polymers *via* Dehydrogenative Direct Alkenylation Polycondensation

Hea Jung Park, Jung Min Joo, Do-Hoon Hwang[*]

Department of Chemistry and Chemistry Institute for Functional Materials, Pusan National University, Korea

Two π-conjugated polymers were successfully synthesized by polycondensation *via* dehydrogenative direct alkenylation with Pd(II) catalyst ($Pd(OAc)_2$) without directing groups in an atom- and step-economical and eco-friendly manner. Using the $Pd(OAc)_2$/pyridine catalytic system, C-H activation of the C-5 position on the thiophene moiety of 3,6-di(thiophen-2'-yl)diketopyrrolopyrrole derivative was regioselective and the cross-coupled products were readily formed with trans-configuration. The optical, electrochemical, and thermal properties of the synthesized polymers were studied to investigate their potential applicability to semiconducting materials.



Poster Presentation : **ORGN.P-455**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

A Study on the Chemoselective Hydroalkoxylation of 2,3,4-Triol Hexopyranosides

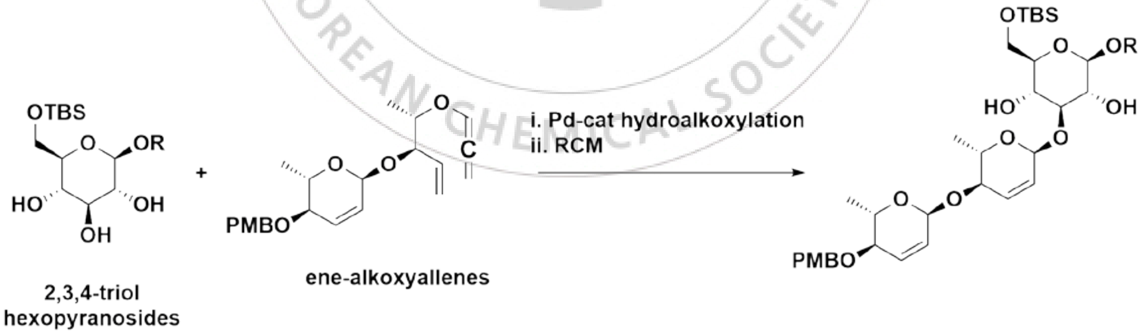
Bhawna Barpuzary, Young Ho Rhee*

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

The regioselective Pd-catalyzed hydroalkoxylation reaction between ene-alkoxyallenes and 2,3,4-triol hexopyranosides is reported.[1] The strategy can provide complex oligosaccharides in high stereoselectivity with no need of protection of hydroxy groups. In this presentation, the optimization of reaction conditions and its potential application for the synthesis of various complex oligosaccharides will be introduced.

References

[1] a) Lim, W.; Kim, J.; Rhee, Y. H., J. Am. Chem. Soc. **2014**, *136* (39), 13618-13621; b) Lee, J.; Kang, S.; Kim, J.; Moon, D.; Rhee, Y. H., Angew. Chem. Int. Ed. **2019**, *58* (2), 628-631.



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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ORGN.P-456**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

A Synthetic Study towards Total Synthesis of 7-Oxostaurosporine by using Palladium-Catalyzed Asymmetric Addition Reaction of Bis-indole to Alkoxyallenes

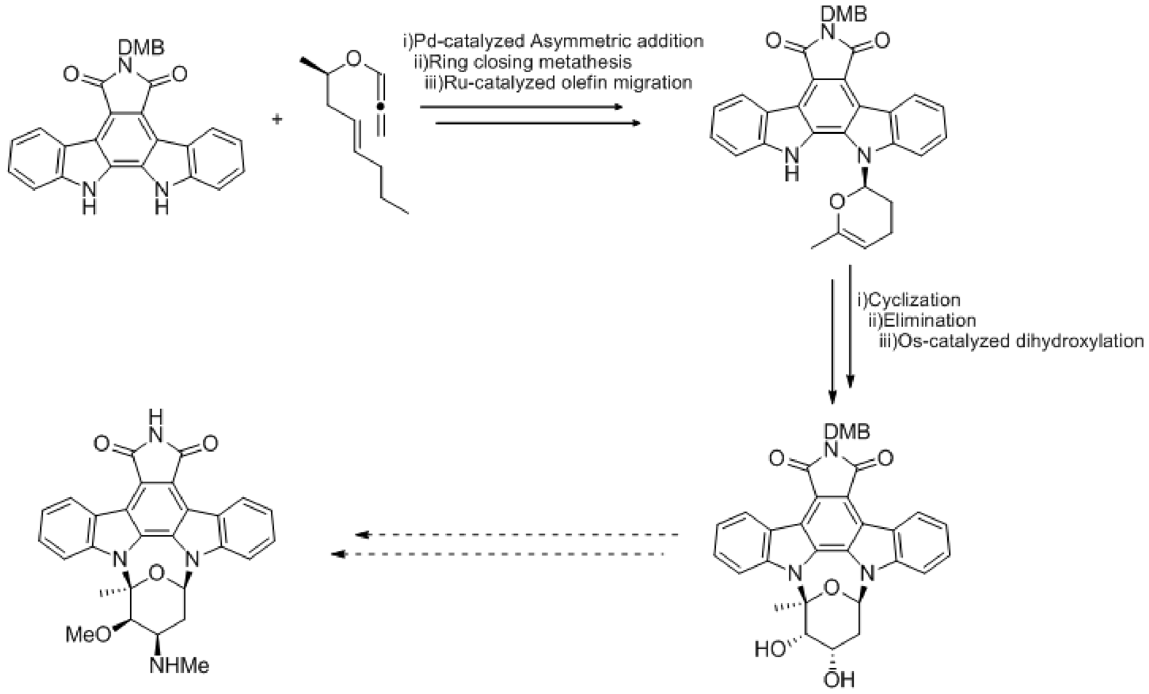
Seok Hyeon Jang, Young Ho Rhee*

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

Staurosporine has interesting biological properties including antifungal and hypotensive activities. Its cytotoxic activity was based on the inhibition of protein kinase C. Herein, a new concise synthetic method towards 7-oxostaurosporine will be presented. Key features of this reaction include i) Palladium-catalyzed asymmetric addition of bis-indole to alkoxyallenes[1], ii) Ruthenium-catalyzed ring closing metathesis(RCM) and iii) Ruthenium-catalyzed olefin migration of cyclic allylic acetal[2]. By using these reactions, Key intermediate of 7-oxostaurosporine could be obtained with high synthetic efficiency.

Reference

1) Jang, S.H. ; Kim, H.W. ; Jeong, W. ; Moon, D. ; Rhee, Y.H., Org. Lett., **2018**, *4*, 1248. 2) Seo, K. ; Kim, Y.J. ; Rhee, Y.H., Org. Lett., **2018**, *4*, 979.



7-Oxostaurosporine

Key intermediate

Poster Presentation : **ORGN.P-457**
Organic Chemistry
Exhibition Hall 1, FRI 11:00~12:30

De Novo Synthetic Approach toward Tetra-saccharides of Cerivimycin

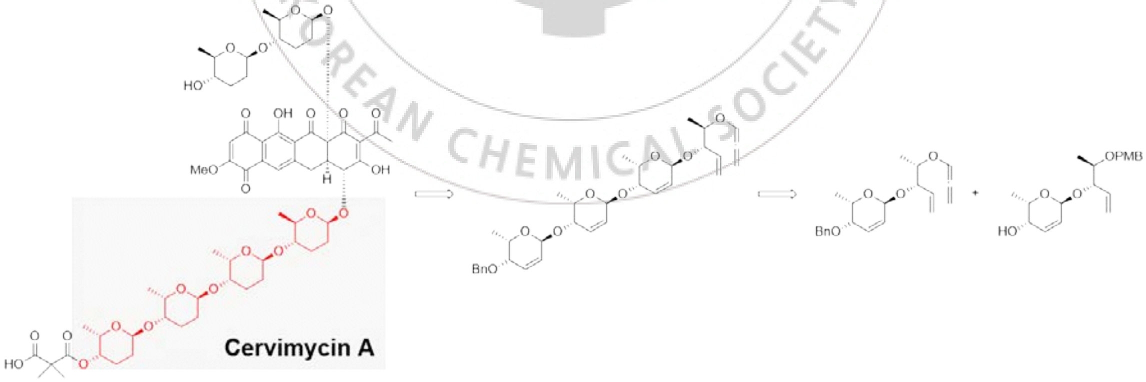
Jihun Kang, Young Ho Rhee*

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

The Cervimycins containing 2,3,6-trideoxy-tetrasaccharide have bioactivity against multi-drug-resistant bacteria. Because of these utilities, Cervimycins have drawn considerable attention from synthetic community. We present here a convergent synthetic study toward tetrasaccharide moiety of Cerivimycin A[1]. Key feature of this strategy is represented by the Pd-catalyzed asymmetric hydroalkoxylation of alkoxyallene which allows for the efficient coupling of the aglycon and the tetrasaccharide moiety.

Reference(s)

1. (a) Lee, J.; Kang, S.; Kim, J.; Moon, D.; Rhee, Y. H., *Angew. Chem. Int. Ed*. **2019**, *58*, 628-631.



Poster Presentation : **ORGN.P-458**

Organic Chemistry

Exhibition Hall 1, FRI 11:00~12:30

[Withdrawal] Palladium Catalyzed Asymmetric Decarboxylative Addition of β-keto acid to alkoxyallene

Sukhyun Lee, Dong-Jin Jang, Young Ho Rhee*

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

Poster Presentation : **MEDI.P-236**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Design and synthesis of Potential SULT4A1 Substrates

Karim El-Baz, Gyo chang Keum[1,*]

Center for Neuro-medicine , University of Science & Technology - Korea Institute of Science and Technology, Korea
[1]*Chemoinformatics Research Center, Korea Institute of Science and Technology, Korea*

Cytosolic sulfotransferases (SULTs) comprise a family of enzymes that catalyze the transfer of a sulfonate group from 3’-phosphoadenosine 5’-phosphosulfate (PAPS) to an acceptor group of various substrates.Consequently, SULTs modulate the activities of a long list of small endogenous and foreign chemicals, including drugs, toxic compounds, steroid hormones, and neurotransmitters. Upon sulfonation, the compounds become more water soluble and hence easily excreted. Among the family, SULT4A1 remains unexplored target with little information about its substrates and sulfate donor. Here within, we report the design of various small molecules with steroidal nucleus and their biological assay in the presence and absence of PAPS as an attempt to reveal some of the characteristics of SULT4A1.

Poster Presentation : **MEDI.P-237**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication and Characteristic Evaluation of Polymer Composite Scaffold Using 3D Bio-Printing

Sang Hyeob Lee, Il Yoon[1,*]

Department of Nanoscience, Nano Drug Delivery Lab, Korea
[1]*PDT Laboratory, Inje University, Korea*

The development of 3D scaffolds using biocompatible polymers is necessary to have advantages suitable for cell proliferation and differentiation by providing an environment similar to a human body. In this study, 3D scaffolds were prepared with a 3D bio-printer using polycaprolactone (PCL), which has good strength and ductility as FDA approved biodegradable polymer. The resulting 3D scaffolds exhibited significantly different size of the pore and strength of the scaffolds, which is the main property of the scaffolds, varied greatly depending on the three printing parameters of pressure, temperature, and velocity. As the pressure and temperature increased, the pore size was decreased and the strength of the scaffolds was increased. However, as the velocity increased, the pore size was decreased and the shape of deformation was occurred, and the strength of the scaffolds was decreased. We confirmed the appropriate parameter conditions for the preparation of 3D PCL scaffolds and these results will be useful information for the development of biodegradable and biocompatible 3D scaffolds using PCL based other polymer composites.

Poster Presentation : **MEDI.P-238**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Water soluble Organic Nano Particles for Effective Drug Delivery in Photodynamic Therapy

Yang Liu[*], **Il Yoon**[1]

Nano Science and Engineering, Inje University, Korea
[1]*PDT Laboratory, Inje University, Korea*

Photodynamic therapy (PDT) is a treatment that uses a drug, called a photosensitizer or photosensitizing agent, and a particular type of light. When photosensitizers are exposed to a specific wavelength of light, they produce a form of oxygen that kills nearby cells. It has some advantages, such as:1)It has no long-term side effects when used properly.2)It’s less invasive than surgery.3)It usually takes only a short time and is most often done as an outpatient.4）It can be targeted very precisely.5）Unlike radiation, PDT can be repeated many times at the same site if needed.This poster presents that (a) synthesis and characterization of new dendritic polymer (2nd generation) type PS contains twelve PSs (methyl pyropheophorbide a) to generate high amount of reactive oxygen species (ROS, such as singlet oxygen) after light irradiation, resulting in enhanced PDT; (b) easy introduction of different PS to cover various wavelength absorption range (red-shift to allow deeper penetration of light in tumor tissue); (c) excellent accumulation in the intracellular and/or extracellular space of tumors (it is not necessary to give a cellular internalization), which is very useful to kill cancer cells especially in vivo based on the enhanced permeability and retention (EPR) effect of nanoparticles; (d) as a future work, 3rd, 4th and 5th generations of dendrimer type PS can make very powerful delivery systems with a large amount of PSs (24, 48, and 96 PSs, respectively) for excellent PDT activity with good water solubility for in vivo as well as clinical trial.

Poster Presentation : **MEDI.P-239**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

QSAR modeling of the acute contact toxicity to honeybees

Young eun Song, Hyung Sik Jo[1], Sung Kwang Lee[2,*]

department of chemistry, hannam university, Korea
[1]*department of chemistry, Hannam University, Korea*
[2]*Department of Chemistry, Hannam University, Korea*

Acute contact bee toxicity is an experiment that evaluates the degree of toxicity by contacting the compound with the bee's thorex. This is an important ecological indicator because of the nature of bees that are the main pollinators in crops, forest and tropical ecosystems. Due as several non-target animals, plant species, are at risk due to the indiscriminate application of pesticides, bee toxicity studies on chemical are needed. But toxicity test is not only time consuming and costly, but it also creates ethical problems. One of the method to solve this problem is the QSAR(Quantitative Structure-Activity Relationship). QSAR model that predict toxicity of untested chemicals are also useful for regulatory purposes. In this study, we developed a QSAR model based on LD50 data to acute contact bee toxicity according to OECD Guideline 214. Toxicity data that collected from US EPA and QSAR Toolbox 4.3, were divided into training set for model learning and external set for validation at a ratio of 6:4. The machine learning method used to construct QSAR model are multiple linear regression(MLR) and support vector machine (SVM), and genetic algorithm that used to select optimal parameters. The developed models were evaluated for predictability and chance correlation using internal/external validation and y-scrambling method. In addition, applicability domain(AD) of model was assigned to specify a reliable predictition range of the model.

Poster Presentation : **MEDI.P-240**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

The effect of butyric acid produced by engineered E.coli on treatment of ulcerative colitis

Young-Tae Park, Taejung Kim, Jungyeob Ham*

Natural Products Research, Korea Institute of Science and Technology, Korea

Butyric acid belongs to short-chain fatty acids (SCFAs) and is the most plentiful metabolite derived from bacterial fermentation of carbohydrates such as dietary fibers in the intestine.Faecalibacterium prausnitzii (FP) is one of the most abundant bacteria in the human intestinal microbiota and regarded as a major effector in human intestinal health because of its anti-inflammatory effects. It produces butyric acid which has beneficial effect on human gut health. However, the extreme oxygen sensitivity has been a major obstacle to cultivate and study physiological characteristics of this organism. The genes encoding Butyryl-CoA dehydrogenase (BCD) and Butyryl-CoA: Acetate-CoA-transferase (BUT) in FP were cloned and expressed in E. coli to determine the effect of butyric acid production on intestinal health. According to the results of butyric acid production in wild-type E. coli expressing BCD, BUT or both, BCD was shown to be essential, while BUT was dispensable, for the production of butyric acid. The anti-inflammatory effects of butyric acid production were tested by administrating these strains into DSS-induced colitis model mice.

Poster Presentation : **MEDI.P-241**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecular Docking Study for Biaryl Sulfate Core Based Hepatitis C Virus NS5A Inhibitor

Jung Woo Park, Byeong Moon Kim[1], Eun-Kyoung Bang[2], Gyo chang Keum[3,*]

Dev. of Data Analysis, Korea Institute of Science and Technology Information, Korea
[1]*Division of Chemistry, Seoul National University, Korea*
[2]*Center for Neuromedicine, Korea Institute of Science and Technology, Korea*
[3]*Chemoinformatics Research Center, Korea Institute of Science and Technology, Korea*

Molecular docking forecasts structure of ligand-protein complexes by modeling protein-ligand interactions at the atomic level based on the structure of the target protein, and can identify how ligands bind within the binding site of the target protein. The rapid development pf X-ray crystallography and NMR technology allowed molecular docking to clearly identify the structural interactions between proteins and ligands. In addition, due to the remarkable development of computer performance and the development of simulation techniques, the accuracy of calculation methods based on structural information has increased, so docking studies are used to develop new drugs.In this study, the target protein was modeled by homology modeling technique, and the molecular docking studies were used to analyze and predict the binding structure between the target protein and the biaryl sulfate core based Hepatitis C virus NS5A inhibitor candidates. In the case of the symmetric inhibitor, it was proved by the calculation that the stabilization of the D-Phenylglycine moiety is reduced due to the π-alkyl interaction between the carbamate methyl group and Tyr93A.

Poster Presentation : **MEDI.P-242**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Studies on the Development of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

Hye Yeon Lee, Haeun Lee[1], WooSeung Son[2], Ae Nim Pae[3], Hak Joong Kim[*], Sang Min Lim[3,*]

Department of Chemistry, Korea University, Korea
[1]*Biochemistry, Korea University of Science and Technology, Korea*
[2]*Department of Chemistry, Yonsei University, Korea*
[3]*Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is the most common form of dementia and becomes a serious problem in modern aging society. Tau is a microtubule-associated protein and is believed to play an important role in AD pathology. In normal condition, tau protein binds to microtubules and helps stabilize neuronal microtubules. However, in pathological state, tau protein is hyperphosphorylated and dissociated from microtubules. These detached tau proteins tend to self-assemble and form oligomers, eventually forming paired helical filaments (PHFs) and neurofibrillary tangles (NFTs). While the need for treatment of AD is increasing, there are drugs that can only alleviate some of the symptoms of AD. Therefore, we pay attention to the hypothesis that tau oligomers are the most toxic form of tau, and intend to develop tau aggregation inhibitors as disease-modifying drug candidates. To find new lead compounds that can inhibit tau aggregation, we performed a high-throughput screening based on a Bi-FC assay with in-house libraries. Thereafter, by modifying hit compounds, we found more potent and less toxic compounds than Methylene blue: a well-known *in-vitro* tau aggregation inhibitor. Currently, we have synthesized various derivatives through a structure-activity relationship study to search for compounds that are more potent than the hit compounds. We are also trying to find potent compounds possessing novel scaffolds by introducing bioisosteres. We will continue our efforts to optimize potency as well as physicochemical properties to develop non-clinical candidates for AD.

Poster Presentation : **MEDI.P-243**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structure-activity relationship of 2,4-disubstituted pyrimidine derivatives as TAM kinase inhibitors

Yeonkyung Lee, Yeonji Kim, Hyunjin Kim[1], Jong Yeon Hwang[1], Pilho Kim[1], Jae du Ha[1], Sang Hun Jung[2], Sung Yun Cho[1,*]

Chungnam National University, Korea
[1]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*
[2]*College of Pharmacy, Chungnam National University, Korea*

The TYRO3, AXL and MERTK (TAM) family of receptor tyrosine kinases (RTKs) are aberrantly regulated in multiple haematological and epithelial malignancies. Rather than functioning as oncogenic drivers, their induction in tumour cells predominately promotes survival, chemoresistance and motility. The unique mode of maximal activation of this RTK family requires an extracellular lipid–protein complex. Recently, it has been reported that Tyro3 target inhibitor is being proposed as a drug target for breast cancer treatment, and that Tyro3 is expressed more strongly in liver cancer than normal tissue, and is important for cancer growth and liver destruction. Regulating the inhibition or overexpression of Tyro3 may be an important target for the development of liver cancer therapeutics. Among the TAM families, there were several adverse effects when Axl and Mer were knocked out, but no specific problems were found when Tyro3 was knocked out. Thus, the development of selective inhibitors of TAM receptors, particularly Tyro3, has attracted attention as a way to overcome the side effects of TAM receptor inhibition. In this report, we synthesized a series of novel series of Aryl or heteroaryl-N4-(piperidin-4-yl)pyrimidine-2,4-diamine derivatives that were substituted with aniline moieties and evaluated for TAM kinase inhibitory activity.

Poster Presentation : **MEDI.P-244**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

An Efficient One-Pot Synthesis of Dibenzoxepino[4,5-c]pyrrole *via* Aldol Condensation and Etherification

Sungil Park, Jung-Nyoung Heo[1,*]

Department of Chemistry, Chungnam National University, Korea
[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Dibenzoxepino[4,5-c]pyrrole is an important scaffold that shows interesting biological activities. Especially, Asenapine (Saphris®) has been used for the acute treatment of schizophrenia and bipolar disorder. Here, we will present a novel and efficient synthetic method *via* sequential intramolecular aldol reaction and S_NAr reaction for diarylether formation. It is noteworthy that the synthesis of the proposed tetracyclic compound could be achieved by a transition metal-free and one-pot reaction under mild conditions.

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Poster Presentation : **MEDI.P-245**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of (2*H*)-Indazoles via Rh(III)-Catalyzed C-H Activation Using Paraformaldehyde

Saegun Kim, Sukhun Lee, In Su Kim[1,*]

School of Pharmacy, Sungkyunkwan University, Korea
[1]*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The indazole core is a ubiquitous scaffold in the field of modern drug discovery. Particularly, (2*H*)-indazoles are crucial pharmacophores found in various bioactive molecules and pharmaceuticals including niraparib and pazopanib. Therefore, much effort has been devoted to the development of methods for the synthesis of (2*H*)-indazoles. To the best of our knowledge, the application of paraformaldehyde as an abundant C1-feedstock to generate C3-unsubstituted (2*H*)-indazoles is unexplored. The method is readily extended to the coupling reaction between azobenzenes and trifluoroacetaldehyde. This transformation efficiently produces a range of C3-unsubstituted and C3-trifluoromethylated (2*H*)-indazoles, which are important targets in the development of novel bioactive compounds. Moreover, (2*H*)-indazoles containing a CF_3 group at the C3-position are considered as pharmacologically privileged scaffolds in drug discovery. Paraformaldehyde has served as a valuable reagent for one-carbon homologation reactions in organic synthesis.

Poster Presentation : **MEDI.P-246**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Direct access to alkyl diazines, Wittig reagents in an unconventional role

Na Yeon Kwon, Dongeun Kim, In Su Kim[1,*]

School of Pharmacy, Sungkyunkwan University, Korea
[1]*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

Alkyl diazines are ubiquitous motifs in medicinal chemistry and natural products. They, as building blocks, are of paramount interest because of their therapeutic potential and broad range of applications including flavors, fragrances, dyes, pesticides, and semiconductors. The direct installation of alkyl group on diazine ring has been rarely explored. Previously studied approaches for the synthesis of alkylated diazines often demonstrate the transition-metal-mediated cross-coupling reactions, Minisci-type alkylations of diazines using radical sources and few others. However, the formation of residual metal wastes and regioisomeric impurities remains an obstacle in the pharmaceutical application. Therefore, an efficient method for the formation of alkylated diazines under metal-free conditions is highly desirable. Herein we report a method for the metal-free site-selective C−H alkylation of diazine-*N*-oxides using wittig reagents to provide a variety of alkylated diazine derivatives, with wide functional group tolerance. As starting materials diazine N-oxides are inexpensive, readily available and could be prepared conveniently. They appear to be favorable replacements of halodiazines as substrate for synthesis of alkyl diazines. Diazine N-oxides were treated with phosphonium ylides under basic conditions to yield alkyl diazines in good yields. The utility of this method is showcased by the late-stage functionalization of a commercially available smoking cessation agent and sequential C−H alkylations of a pyrazine-*N*-oxide to provide the corresponding 2,3-dialkyl pyrazine. Hence, this method has great potential for applications in medicinal chemistry research

Poster Presentation : **MEDI.P-247**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

A Novel Orally Active Inverse Agonist of Estrogenrelated Receptor Gamma (ERRg), DN200434, A Booster of NIS in Anaplastic Thyroid Cancer

Jina Kim, Sangbong Lee, Jungwook Chin, Sung Jin Cho*

New Drug Development Center, DGMIF, Korea

New strategies to restore sodium iodide symporter (NIS) expression and function in radioiodine therapy–refractive anaplastic thyroid cancers (ATCs) are urgently required. Recently, we reported the regulatory role of estrogen-related receptor gamma (ERRg) in ATC cell NIS function. Herein, we identified DN200434 as a highly potent (functional IC_{50} = 0.006 mmol/L), selective, and orally available ERRg inverse agonist for NIS enhancement in ATC.

Poster Presentation : **MEDI.P-248**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

Development and structure-activity relationship study of SHP2 inhibitors

Bohee Kim, Seungjin Jo[1], Jeong-Hun Sohn, Byumseok Koh[2], Inji Shin[3,*]

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[1]*University of Science & Technology, Korea*
[2]*Korea Research Institute of Chemical Technology, Korea*
[3]*Department of Fine Chemistry, Seoul National University of Science & Technology, Korea*

SHP2 known as the non-receptor protein tyrosine phosphatase encoded by *PTPN11* gene has an important role in the control of cell growth and differentiation. It has been identified that activating mutations of SHP2 related to various disease, such as Noonan syndrome and various cancers, including leukaemia, lung and breast cancer. Therefore, the discovery of SHP2 inhibitors can be important to treat of cancers. High-throughput screening (HTS) was performed using more than 10,000 compounds from Korea Chemical Bank and a hit compound with 94 nM of IC_{50} value was obtained. We have designed and synthesized new derivatives of a hit compound to explore the structure-activity relationship (SAR) study. Biological activity was also studied in MDA-MB-468 cell line associated with a breast cancer.

Poster Presentation : **MEDI.P-249**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

Novel Hypoxia-Inducible Factor 1α (HIF-1α) Inhibitors for Angiogenesis-Related Ocular Diseases: Discovery of a New Scaffold via Ring-Truncation Strategy

Hongchan An, Young Ger Suh[1,*]

Daegu Gyeongbuk Medical Innovation Foundation, Korea
[1]*Seoul National University, Korea*

Ocular diseases featuring pathologic neovascularization are the leading cause of blindness, and anti-VEGF agents have been conventionally used to treat these diseases. Recently, regulating factors upstream of VEGF, such as HIF-1α, has emerged as a desirable therapeutic approach because the use of anti-VEGF agents is currently being reconsidered due to the VEGF action as a trophic factor. Here, we report a novel scaffold discovered through the complete structure-activity relationship of ring-truncated deguelin analogs in HIF-1α inhibition. Importantly, the heteroatom-substituted benzene ring as a key structural feature of the new analog, was identified as a novel scaffold for HIF-1α inhibitors that can be used in lieu of a chromene ring.

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Poster Presentation : **MEDI.P-250**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Microwave-assisted deglycosylation of korean mistletoe improved tyrosinase inhibition

Jaehyun Kim, Kooyeon Lee[*], Jung Won Choe, Hakhyun Kim

Department of Bio-Health Technology, Kangwon National University, Korea

The abnormal regulation of melanin synthesis leads to a wide range of pigmentary disorders. Although various melanin biosynthesis inhibitors have been developed, their efficacy and long-term safety needs to be further improved, and thus the goal of this study is to develop promising natural compound inhibitors of melanin biosynthesis. Here, we obtained aglycone flavonoid extract through the microwave-assisted hydrolysis of glycoside extract from Korean mistletoe in acidic condition. The aglycone extract inhibited tyrosinase activity more efficiently with better antioxidant activity than glycoside extract in vitro. The microwave-assisted aglycone extract of mistletoe was further analyzed for in vivo activity, and the results showed the aglycone extract inhibited both early melanocyte development and melanin synthesis more efficiently in zebrafish embryo in a dose-dependent manner. Our in vivo toxicity assay quantitatively measured cell death in zebrafish embryos and showed that the microwave-assisted aglycone extract of mistletoe had no significant effect on cell death ($p < 0.001$), indicating that aglycone extract is more biocompatible than glycoside extract. Furthermore, our in vitro and in vivo analyses successfully identified and characterized velutin, an aglycone of a homoflavoyadorinin B glycoside, as a major inhibitory component in the microwave-assisted mistletoe extract. Ultimately, this study showed that the novel natural compound inhibitor velutin, which was generated through microwave-assisted extraction from mistletoe, improved the efficacy of melanin biosynthesis inhibition with little toxicity.

Poster Presentation : **MEDI.P-251**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Anti-BACE compounds from the Chinese and Korean Propolis

Kayoung Shin, Jintaek Oh, Byong Wook Choi[*], Bong Ho Lee[*]

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Beta amyloid cleaving enzyme(BACE) has been emerged as a new target for developing anti Alzheimer's disease drug. In our continuing search for anti-BACE compounds from various sources, the Korean and Chinese propolis were examined and here we report the progress on the purification and anti-BACE activity. The Korean propolis MeOH extract and, CHCl$_3$, BuOH factions showed 100%, 97.69%, and 97.88% respectively BACE inhibitory activites at 1mg/mL. The Chinese propolis extract and fractions also showed very good BACE inhibitory activities. TEO samples did not showed much difference in BACE inhibitory activity. All of the MeOH extracts and gractions showed dose dependencies. We were able to isolate kaempferol and ferulic acid from the two propolis samples.

Poster Presentation : **MEDI.P-252**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Carbapenem-based fluorogenic substrate for detection of pathogenic carbapenemase-expressing bacteria

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Carbapenem is one of effective antibiotics in treating infections of Gram-negative bacteria due to its high activity against a broad range of bacterial pathogens and excellent stability to most β-lactamases. However, the emergence of carbapenem-resistant enterbacteriaceaes (CREs) is spreading around the world at an alarming rate. Thus, the risk of carbapenem resistance is increasing and becoming a major public health threat in many countries.One of the important causes of carbapenem-resistance is carbapenemase-producing organisms (CPOs), which specifically acquire and express carbapenemases that cleave the amide bond of the crucial β-lactam ring of carbapenem antibiotics. Therefore, efficient and accurate detection of carbapenemase-producing CREs (CP-CREs) is necessary for the management and ongoing treatment of infection.Current methods of detecting CP-CREs can be classified into phenotypic and genotypic methods. Although the phenotypic methods are widely used for clinical purpose due to their cost effectiveness, they are time consuming and lack sensitivity and specificity compared to the genotypic methods. Recently, activity-based detection methods have been developed to overcome these shortcomings. In particular, a fluorescent-based screening method has received much attention due to its low cost, high sensitivity and simplicity.In this study, we describe the synthesis of a novel fluorescent carbapenemase substrates and their evaluation for detection of CP-CREs. These probes include a β-lactam component of carbapenem structure as an enzyme recognition site, ethereal likers as a cleavage site, and fluorescence dyes as a signal producer. The preliminary results from enzyme assay of our probes indicated that several substrates showed good specificity and selectivity to a series of carbapenemases which will be further investigated for detection of the CP-CREs in clinical samples.

Poster Presentation : **MEDI.P-253**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Reduced-Lipoic acid (Dihydrolipoic acid; DHLA) Derivatives for Butyrylcholinesterase Inhibitor

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Acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) inhibitors are well known as a drug target for Alzheimer's disease. Under certain conditions, α-lipoic acid was unstable and many side reactions occurred such as rings open and polymerization reactions. To overcome this problem, the disulfide bonds in lipoic acid were reduced to dithiol functional group. Dihydrolipoic acid (DHLA) is the reduced form of lipoic acid (LA). In this study, a series of thioactal compounds were synthesized using the DHLA of compound A and various aldehyde compounds and the inhibitory effects on AChE and BuChE were investigated. The cholinesterase inhibitory activity (IC_{50}) of compound A were 88.3 uM for AChE and 4.0 uM for BuChE. In general, IC_{50} value of thioactal compounds did not get better than the starting compound A. Compound 1 (IC_{50} = 3.39 uM for BuChE) showed a little bit better inhibitory activity than the starting compound A and the positive control compound, galantamine (IC_{50} = 9.4 uM for BuChE).

Poster Presentation : **MEDI.P-254**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

Discovery of highly selective csf1r inhibitors.

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Colony stimulating factor-1 receptor (CSF-1R) belongs to class III Receptor Tyrosine Kinase (RTK), it has been reported that CSF1R is related to cancer, autoimmune disease and bone disorder. Therefore, CSF-1R has been considered as an attractive target for cancer and autoimmune disease.CSF-1R inhibitors have been developed. Currently, one CSF-1R inhibitor (Pexidartinib) was approved by FDA in 2019. However, more selective, potent CSF-1R inhibitor for diverse indications is still required.Herein, we described novel and selective CSF-1R inhibitors designed and synthesized inhibitors with heterocyclic scaffold. Their activities were evaluated in cell viability test and cell free kinase assay. A representative compound showed 15nM of IC50 in cell free kinase assay. Further investigation is in progress to analyze structure-activity relationship and to find a high quality lead.

Poster Presentation : **MEDI.P-255**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

High throughput oligonucleotide sandwich assay for genomic biomarker detection in prostate cancer

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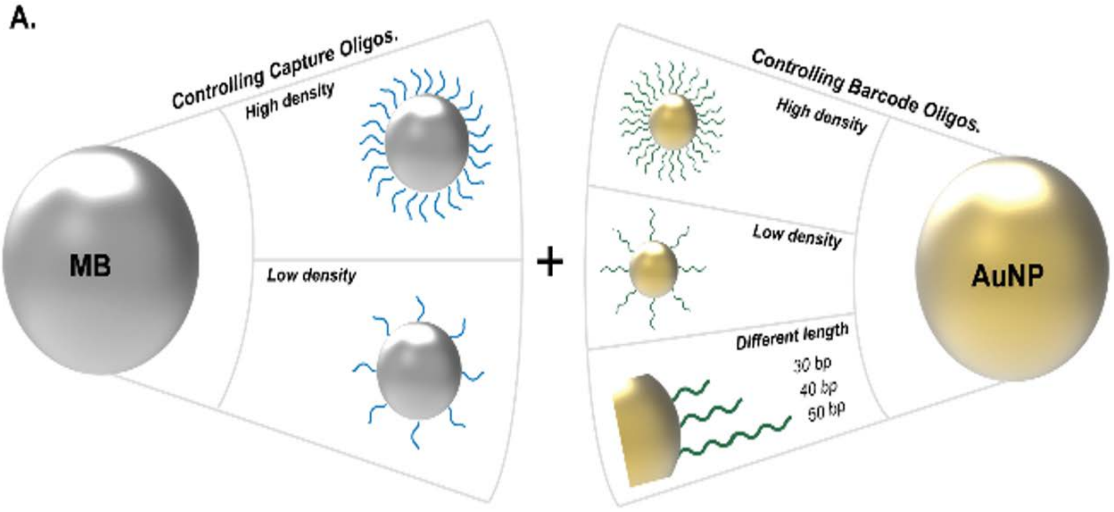
Prostate cancer is one of the leading causes of death in American men. The prostate-specific antigen test has been employed in clinics for the diagnosis of prostate cancer using patients' blood samples. However, the low sensitivity and low accuracy of this test lead to misdiagnoses. As an alternative, genomic biomarker detection technique such as oligo-sandwich assay has been gaining significant attention due to its high sensitivity and multiplexing capability. Although the oligo-sandwich system has previously demonstrated its efficacy in other cancer detection from patient blood samples, an improved system with high sensitivity is necessary for prostate cancer detection from patients' non-invasive bio-fluid such as urine. Here, we report the fabrication of the oligo-sandwich assay with improved detection level, allowing diagnosis in spiked urine. We simultaneously detected protein biomarkers (AMACR, PCA3, and PSMA) upregulated in prostate cancer tissue. In this method, the target gene couples the magnetic beads (MBs) conjugated with complementary oligos and gold nanoparticles (AuNPs) with tractable sequence (barcode). Varying the initial concentration of capture-oligos in the reaction, we achieved a constant conjugation efficiency of ~ 25% in the number of capture-oligos conjugated per MB. We assessed the influence of the final salt concentration during the salt-aging process (conjugation efficiency in the range of 50-85%) for the effective regulation of barcode-oligos on AuNPs. We also discovered that the length of the overlapping base pairs between targets and oligos is critical for the specificity of the system. Our improved oligo-sandwich platform can be utilized as a powerful non-invasive tool to diagnose prostate cancer in clinics worldwide.



Scheme 1. Schematics of the oligonucleotide sandwich assay

Poster Presentation : **MEDI.P-256**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Solid-phase Parallel Synthesis of 2,4,5-thiazole Derivatives Based on Peptidomimetics

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Department of Chemistry, Dongguk University, Korea

Synthesis of peptidomimetics has known to be effective for better understanding of protein aggregation which causes neurodegenerative diseases such as Alzheimer’s disease and Parkinson’s disease. In this work, solid-phase synthesis of 2,4,5-thiazole derivatives based on peptidomimetics is described. The synthetic strategy starts from constructing ethyl 2-(benzyl(methyl)amino)-4-nitrothiazole-5-carboxylate core skeleton resin with 2-bromo-3-nitroacetophenone. The resulting core skeleton resin undergoes hydrolysis of carboxylate group to afford amide coupling sites for three connected amino acids. Reduction of nitro group is followed to afford amino group for the other tripeptide. Trifluoroacetic acid (TFA) in dichloromethane (DCM) cleavage cocktail is used for removing the resin. The final product has core skeleton of 2,4,5-thiazole with two sets of three consecutive amino acids.

Poster Presentation : **MEDI.P-257**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Hypoxylonol F Isolated from Annulohypoxylon annulatum regulates pancreatic β-cell metabolism to improve insulin secretion.

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Insulin plays an important role in glucose constancy and is used to treat hyperglycemia in diabetes. Annulohypoxylon annulatum is an inedible ball-shaped wood-rotting fungus, and hypoxylon F is one of the major compounds of A. annulatum. The aim of this study is to evaluate the effects of hypoxylonol F on insulin secretion in INS-1 pancreatic β-cells and demonstrate the molecular mechanism involved. Glucose-stimulated insulin secretion (GSIS) values were evaluated using a rat insulin ELISA kit. Moreover, the expression of proteins related to pancreatic β-cell metabolism and insulin secretion was evaluated using Western blotting. Hypoxylonol F was found to significantly enhance glucose-stimulated insulin secretion without inducing cytotoxicity. Additionally, hypoxylonol F enhanced insulin receptor substrate-2 (IRS-2) levels and activated the phosphatidylinositol 3-kinase/protein kinase B (PI3K/Akt) pathway. Interestingly, it also modulated the expression of peroxisome proliferator-activated receptor (PPAR) and pancreatic and duodenal homeobox 1 (PDX-1). Our findings showed that A. annulatum and its bioactive compounds are capable of improving insulin secretion by pancreatic β-cells. This suggests that A. annulatum can be used as a therapeutic agent to treat diabetes.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **MEDI.P-258**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Design and evaluation velutin derivatives for investigation of molecular structure and its inhibitory effect against tyrosinase activity.

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Department of Bio-Health Technology, Kangwon National University, Korea

Velutin, a flavonoid aglycone extracted from Korean mistletoe, has potent inhibitory activity against melanin biosynthesis through inhibiting tyrosinase activity. However, the role of four functionalities on flavonoid backbone in regulation of tyrosinase activity has not been clearly understood. In this study, to investigate relationship between velutin structure and its inhibitory effect against tyrosinase activity, we designed and synthesized 12 derivatives by modifying four functional sites with hydrogen, hydroxyl, and methoxy functionalities. We evaluated inhibitory effect of 12 derivatives on tyrosinase activity through determining amount of dopachrome produced by tyrosinase. While substitution of hydroxyl (C-5) and methoxy (C-7) group with other functionalities in A ring of flavonoid backbone changed its inhibitory effect, substitution of hydroxyl (C-4) and methoxy group (C-3) with other functionalities in B ring had no significant effect, indicating that molecular structure of A ring is closely related with inhibitory effect. Taken together, this study would be helpful for development of drug to treat dysregulation of melanogenesis.

Poster Presentation : **MEDI.P-259**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Protective effect of hypoxylonol C and BNT against streptozotocin induced damage in INS-1 cells.

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The number of people with diabetes mellitus has been increasing in the last few decades, and it is now recognized as a global public health problem. The loss and dysfunction of pancreatic β-cells is the key feature of diabetes. Loss of pancreatic β-cell function leads to insulin deficiency, which then results in hyperglycemia. Natural product extracts and their compounds are more attractive than synthetic drugs as drug candidates, as synthetic drugs treat the primary symptoms of a specific disease as understood by scientific pathology, whereas natural products usually act by healing and repairing body functions that are affected by the primary symptoms. This encourages the development of many natural compounds that have biological potency. In recent decades, interest in the production of secondary metabolites from mushrooms has increased due to their various biological activities. Among these, Annulohypoxylon annulatum a ball-shaped wood-rotting fungus that contains unique benzo[j]fluoranthene compounds, which protect against cisplatin-induced renal proximal tubular damage, and inhibits tumor angiogenesis. However, the anti-diabetic effects of A. annulatum mediated by the improvement of pancreatic β-cell function have not yet been elucidated. Here, we investigated the protective effects of A. annulatum and its compounds on STZ-induced pancreatic β-cell dysfunction and their underlying molecular mechanism in INS-1 cells.

Poster Presentation : **MEDI.P-260**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Comparison and Expectations of Drug Tests in 3D Printing Bioink with *In vitro*, *In vivo*Test.

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Conduct an in vitro, in vivo to test the toxicity or efficacy of a drug.The results of the in vitro test can be different from 3D.In vivo tests often produce results that are different from those of clinical trials. Because of this, bioink using a 3D printer is used in a 3D environment, highlighting the advantages and mitigating shortcomings of the in vitro as well as in vivo tests.Bioink using a 3D printer can solve both the disadvantages of in vitro and in vivo tests. because it uses a scaffolds with the same data in 3D environment.After cultivating cancer cells by mixing alginate, agarose, collagen, and gelatin as the materials to be used in bioink for checking drug effect.

Poster Presentation : **MEDI.P-261**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and Biological Evaluation of Potent β-Arrestin-biased S1P1 Agonist for Multiple Sclerosis Treatment

Jee yun Ahn, WooSeung Son[1], Hyeon Jeong Kim, Kyu-Sung Jeong[1], Jong-Hyun Park, Ki Duk Park, Sang Min Lim, Ae Nim Pae[*]

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Multiple sclerosis is a T-cell related autoimmune disease of the central nervous system. FTY720 (Fingolimod) is the first FDA-approved orally available drug for relapsing remitting MS. In clinical trials, it had side effects such as bradycardia and hypertension. Our goal is discovery potent and selective Sphingosine-1-phosphate receptor 1 (S1P1) agonist for being lower the circulating lymphocytes more efficiently by internalization of receptor on lymphocyte. We designed and synthesized S1P1 receptor agonists with selectivity against S1P3 receptor, which may result in heart-related diseases, via in silico docking study on S1P1 receptor crystal structure. S38, the lead compound, showed remarkable in vitro activities with sparing activity against S1P3 receptor. Further compounds were synthesized for improving solubility in buffer for peripheral lymphocyte counting assays. A61 and A63 exhibited good solubility as well as excellent in vitro activities (β-arrestin assay EC50= 9.2 nM and 6.9 nM, respectively). However, the compounds was observed poor ADME properties. The optimization of novel S1P1 agonist to maintain good solubility with enhanced potency and ADME properties is now in progress.

Poster Presentation : **MEDI.P-262**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Discovery of Novel tau aggregation inhibitors 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 unknown what AD causes, but AD features two histopathological hallmarks : amyloid plaques(AP) made of amyloid-β and neurofibrillary tangles(NFTs) arising from the hyperphosphorylated tau aggregation in pathology. It is known AP and NFT are neurotoxic that may lead to impairment of brain. In clinical trials, several compounds, such as amyloid aggregation inhibitors, β-secretase inhibitors and so on, have been failed to cure AD patients. Therefore, our rationale of tau aggregation inhibitors block aggregation of hyperphosphorylated tau protein that may cause AD. We identified lead compound (DTC0100) which inhibits tau aggregation by high throughput screening in Tau Bi-FC cell-based assays. Then, a variety of derivatives were synthesized through a structure-activity relationship study and the optimization of novel tau aggregation inhibitors to improve potency, physicochemical properties and in vivo efficacy. Among synthesized compounds, DTC0521 showed excellent inhibitory activity of tau aggregation (IC50 = 0.06 μM) in Tau Bi-FC assays and was lower tau aggregation (IC50 = 0.58 μM) in ThS assays as well. DTC0521 recovered from cognitive impairments (Tau-P301L-BiFC transgenic mice) in behavior test and decreased tau aggregation as well as phosphorylated tau. It also exhibited good pharmacokinetic profile and ADME/Tox, thus, the validation of DTC0521 as preclinical candidate and further optimization are in progress.

Poster Presentation : **MEDI.P-263**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Discovery of Novel β-arrestin-biased S1P1 Agonists for Treatment of Multiple Sclerosis

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Multiple sclerosis (MS) is a chronic, progressive autoimmune disease which causes demyelination of the CNS. The non-selective Sphingosine-1-phosphate (S1P) receptor modulator, FTY720, binds to S1P1, 3, 4, 5. In Human clinical trials, it is associated with diverse side effects such as hypertension by S1P3 agonism. 1 Our rationale of developing novel selective S1P1 receptor Agonist is to be lower the circulating lymphocytes more efficiently by internalization of S1P1 on lymphocyte. 2 We designed and synthesized S1P1 receptor agonists with selectivity against S1P3 receptor via in silico docking study on S1P1 receptor crystal structure. The synthesized compound KKPS0075 showed remarkable in vitro activities (Ca2+ signaling assay, EC50=23 nM, β-arrestin assay, EC50=1.98 nM and Internalization assay, EC50=0.65 nM) with sparing activity against S1P3 receptor. Furthermore, the compound KKPS0073 show β-arrestin biased signaling as S1P1 agonist(Ca2+ signaling assay, EC50=111 nM, β-arrestin assay, EC50=0.17 nM and Internalization assay, EC50=5.04 nM). Optimization of pharmacokinetic properties and in vivo study is ongoing.

Poster Presentation : **MEDI.P-264**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

KR-26827, a novel and selective anti Zika virus agent based on the 1,2,4-oxadiazole scaffold

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Zika virus (ZIKV), a mosquitoes-associated pathogen is an ascended global health concern over the recent years. The ZIKV transmission has a rapid geographic expansion through humans and mosquitoes and is associated with severe neurological disorders such as Guillain‒Barre syndrome and fatal microcephaly. However, In the absence of selective ZIKV antivirals, the patients have to rely on the broad spectrum antivirals. Thus there is a unmet demand for the development of selective ZIKV antivirals for the treatment of ZIKV infections. Herein we report the discovery of selective anti-ZIKV agents based on 1,2,4-oxadiazole scaffold. High throughput screening with a chemical library gave us several hit compounds with micromolar anti-ZIKV activities. Further optimizations to improve potencies of the given compounds finally provided KR-26827 as our lead compound. Detailed SAR studies will be presented showing KR-26827 as a promising lead with an improved potency, selectivity, promising drug like and physicochemical properties.

Poster Presentation : **MEDI.P-265**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Discovery of zinc-dependent deacetylase LpxC inhibitors against gram-negative bacteria

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Since the discovery of the penicillin, a large number of antibiotics have been employed for the treatment of various bacterial infections in humans. However, over the time the deaths from bacterial infections have increased due to emergence of multidrug resistant bacterial strains. Especially the gram-negative bacteria offer much challenge in the antibacterial drug discovery, because of gram-negative bacteria comprises an outer membrane, which is more complex than the gram-positive bacteria. The Zinc-Dependent UDP-3-*O*-acyl-*N*-acetylgulcosamine deacetylase (LpxC) is an essential enzyme of lipid A biosynthesis in gram-negative bacteria. Previously reported hydroxamate containing compounds showed potently inhibitory activity against LpxC, further development was halted due to poor pharmacokinetic properties. We are currently developing non-hydroxamate inhibitors of LpxC

Poster Presentation : **MEDI.P-266**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Phage display based development of melamine specific bindable bioreceptors, and their verification by melamine mediated GOQD-Hg^{2+} quenching system

Feng Shuaihui, ChanYeong Park, Shi Rongjia, Seung Hoon Baek, Tae Jung Park*

Department of Chemistry, Chung-Ang University, Korea

The blend of melamine to foodstuffs is prohibited, but regardless of its harmfulness melamine contamination to dairy products still occur to cheat their nutritional components. In this study, to find out the bioreceptor recognizing melamine, phage display technology was introduced. For the technique, 2 types of hapten and 2 kinds of phage display kit (both 7-mer and 12-mer PhD Phage-displayed Peptide Library kit) were used to improve its specificity by cross-checking each discovered sequence. Starting from the 2-chloro-4,6-diamino-1,3,5-triazine as an epitope site, 6-aminohexanoic acid is reacted to synthesis hapten. Moreover, the hapten was decorated on the bovine serum albumin as a carrier material to produce BSA-hapten. The phage-displayed peptides are identified by sequencing, analogous and repeated five candidates were selected. After that, their selectivity and affinity against the melamine were verified by graphene oxide quantum dot (GOQD)-Hg^{2+} quenching system. The nitrogen atoms in melamine could coordinate with Hg^{2+} ion, and this melamine-Hg^{2+} complex makes easy to attach on the surface of GOQD through the π-π stacking between melamine and GOQD. As a result of this approach, the fluorescence of GOQD is quenched due to charge transfer. If the screened peptides have an affinity to melamine, the diminished fluorescence intensity will be recovered in consequence of hindering the formation of the melamine-Hg^{2+} complex. Among the five peptides, four peptides represent the affinity to the melamine with a low detection limit even in the pretreated milk sample (9.5 ppm). In this respect, it was revealed that these sequences have applicability for the electrochemical and colorimetric sensors to the melamine.

Poster Presentation : **MEDI.P-267**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Sensitive and selective "turn-on" strategy for fluorescence detection of histamine based on Phage display derived peptide and carbon quantum dots

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Histamine is mostly found in spoiled food and often as a criterion of food safety. Here, our work present a sensitive and selective flurescence detection method for the detection of histamine based on phage display derived peptides and carbon quantum dots. Firstly, a serious of peptides which can specifically binded with histamine were screened by phage display. After that, the N-acetyl-L-cysteine capped fluorescent carbon quantum dots (NAC-CQDs) were synthesized by one-pot hydrothermal treatment and the fluorescence of NAC-CQDs could be effectively quenched by peptides via the electron transfer interactions from NAC-CQDs to peptides due to the electrostatic attraction of NAC-CQDs/peptides complex. In the presence of histamine, peptides have an affinity of histamine so the combination of peptides and NAC-CQDs would be dissociated, leading to the fluorescence recovery of NAC-CQDs. Hence, it was successfully adapted for the detection of histamine in many food such as tuna flesh samples.

Poster Presentation : **MEDI.P-268**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

Lead optimization of the anti-cancer agents inhibiting aminoacyl-tRNA synthetase

Yoojin Park, Eunhye Lee, Seri Bae, Soong-Hyun Kim, Ga Young Park, Eun Bi Ko, JiHee Kang, Youjeong Choi, Minsoo Song*

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Laminin is a major component of the extracellular matrix (ECM) and plays a key role in cell migration, differentiation, and adhesion. Laminin binding to receptors such as integrins and laminin receptor (67LR) activates a signaling pathway for cell migration. In various types of cancer cell lines, 67LR is highly expressed in the cell membrane and induces laminin-dependent cancer cell migration. Recently, the Kim group demonstrated that lysyl-tRNA synthetase (KRS), a crucial enzyme for protein synthesis in the cytosol, is also overexpressed in various kinds of cancer and is translocated to plasma membrane upon laminin signal, consequently stabilizing 67LR and facilitating cancer cell migration in the course of metastasis. Because metastasis is the primary cause of death related to cancer, new therapeutic targets to control metastasis are a hot research topic. Therefore, inhibition of the pro-metastatic interaction of KRS with 67LR has been proposed to be a potential target for the treatment of cancer metastasis.Our medicinal chemistry works have focused on the optimization of initial lead compound BC-KI-00053 that possesses toxicity liabilities. We have identified a potential toxicophore in BC-KI-00053 using in vitro cell tox assay through systematic SAR analysis. Our on-going efforts to develop a small molecule preclinical candidate for inhibiting KRS induced cancer cell migration are described here.

Poster Presentation : **MEDI.P-269**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Design, Synthesis and Biological evaluation of Novel non-covalent Keap1-Nrf2 PPI inhibitors

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The nuclear factor E2-related factor 2 (Nrf2)-Kelch-like ECH-associated protein 1 (Keap1) signaling pathway is involved in cell homeostasis, redox, and regulation of inflammation. Keap1 is a negative regulator of the transcription factor Nrf2 and it induces ubiquitination and proteasomal degradation of Nrf2 under unstressed conditions. Upon oxidative stress, modification of the cysteine residues of keap1 disrupts the Keap1-Nrf2 interaction. Activated Nrf2 then binds to the *cis*-acting antioxidant response element (ARE) site and regulates the expression of numerous cytoprotective, anti-inflammatory and antioxidant enzymes. Thus, activating Nrf2 may have therapeutic effects on many chronic diseases, neurodegenerative diseases, and inflammatory diseases. Recently, direct inhibiting of Keap1-Nrf2 protein-protein interaction (PPI) with non-covalent small molecules is considered a promising strategy to activate Nrf2. To date, several non-covalent small molecule inhibitors have been found. In this study, we designed and synthesized a new non-covalent small molecule compounds based on the previous known compounds by structure-based drug design. We will continue to modify the structure to find potent Nrf2 activators.

Poster Presentation : **MEDI.P-270**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Lead optimization of triple reuptake inhibitor to treat attention deficit hyperactivity disorder (ADHD)

JIhee Kang, Seri Bae, Ga Young Park, Eun Bi Ko, Chunyoung Im, Eunhye Lee, Yoojin Park, Youjeong Choi, Soong-Hyun Kim, Minsoo Song*

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Attention deficit hyperacitivity disorder (ADHD) is neuropsychiatric syndrome that represents inattention, hyperactivity and impulsivity as core symtoms. While the exact cause of ADHD development is unclear yet, stimulant medications (e.g. methylphenidate, amphentamine) and nonstimulant medications (e.g. atomoxetine, clonidine, guanfacine) have been used to alleviate core symtoms of ADHD. Due to the adverse CNS, cardiovascular and gastrointestinal effects of these current treatments, other new approaches for ADHD have been studied in clinical trials. The most advanced clinical study is about centanafadine, targetting inhibition of triple (serotonin-norepinephrine-dopamine) reuptake transporters.In order to develop triple reuptake inhibitor (TRI), we have designed new scaffold of small molecule TRI for ADHD. Over 170 compounds were synthesized and their biological activity were tested by in vitro enzyme assay. Our lead compound, TN-04, showed potent triple reuptake inhibitory activity in vitro (IC50 248, 386, 415 nM, DAT, NET, SERT, respectively). Also, TN-04 demonstrated comparable PK properties to centanafadine, and better efficacy in several mouse behavior model. For instance, TN-04 significantly decreased hyperactivity, impulsivity, and inattention in dose dependent manner in vivo behavior assays using MK-801 model (5, 10, 20 mpk, ip). Our efforts to generate preclinical candidates of TRI for ADHD will be presented.

Poster Presentation : **MEDI.P-271**

Medicinal Chemistry

Exhibition Hall 1, THU 11:00~12:30

Discovery of Novel Kelch-like ECH-Associated Protein 1 (Keap1)-Nrf2 Interaction Inhibitors for Neurodegenerative Disease

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Activation of Nrf2 can be intended to the cellular defending mechanism and induce the expression of about 250 genes that contain cytoprotective genes. Keap1 (Kelch-like ECH-associated protein) is the primary regulator of Nrf2. Protein-protein interactions (PPIs) govern various vital biological processes in normal and disease states, including cell division, adaption, or response to extracellular signals. The direct targeting Keap1-Nrf2 protein-protein interaction has been an effective strategy for Nrf2 activation. We performed FDA approved drug or fragment library screening against fluorescent-based techniques, fluorescence polarization (FP) assay. Seven compounds inhibited Keap1-Nrf2 interaction with IC_{50}'s of less than 10 μM. Docking study suggested that some compounds are a hydrogen bond with Arg415 in the hinge region. We investigated the optimization process for these compounds. Our study provides the potential development of novel Keap1-Nrf2 interaction inhibitors.

Poster Presentation : **MEDI.P-272**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

A progress in discovery of an inhibitor for 53BP1 tandem Tudor domain

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Double-strand break damage of DNA in cell is repaired in two different pathways; non-homologous end joining (NHEJ) and homologous recombination (HR). NHEJ corrects the DNA damage by joining the compatible ends of the broken DNA, but this mechanism frequently connects mismatched pairs of the damaged termini. For this reason, the NHEJ pathway leads to indel mutations which losing some sequence information and even generates chromosomal translocation. In contrast, in the HR pathway, an intact sister chromatic sequence is used as a template enabling the accurate damage repair. The genome editing techniques including CRISPR/Cas9 relies on these two endogenous DNA repair mechanisms. In genome editing campaigns, the ratio between HR and NHEJ pathways determines the outcome leading to either a precise knock-in of a specific DNA sequence or a simple gene disruption, respectively.53BP1 is a key factor to promote the NHEJ pathway over HR by forming a barrier to prevent excessive resection. The recognition of dimethyl state of histone 4 lysine 20 (H4K20me2) near the breakage site by a tandem Tudor domain of 53BP1 was shown to be a key step in this process. This information led us to hypothesize that discovery of a potent inhibitor for tandem Tudor domain of 53BP1 would enable precise gene knock-in during genome editing by suppressing the NHEJ pathway and thereby directing the DNA repair pathway towards the HR pathway. This poster presentation will summarize our recent efforts to discover a new inhibitor for 53BP1 tandem Tudor domain based on thermal shift assay-based fragment screening.

Poster Presentation : **MEDI.P-273**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Identification of new potent anticancer 7-deazapurines with dual induction of apoptosis and TrkA inhibitory activities

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Tropomyosin-related kinase A (TrkA) plays important roles in tumor cell growth, survival signaling, and chemo-resistance in pancreatic cancer. Through our extensive SAR exploration of several 7-deazapurines as anticancer agents, KK5101 was developed as a novel selective TrkA inhibitor with potent antiproliferative activity against several cancer cell lines. Further biological studies of KK5101 disclosed its ability to inhibit the proliferation of pancreatic cancer cells MIAPaCa-2 and PANC-1. In addition, KK5101 activated the process of apoptosis, associated with loss of mitochondrial membrane potential, increased cleaved caspase-3 and PARP levels and numbers of TUNEL-positive apoptotic cells. Annexin-V assay showed that KK5101 increases cell death including early and late apoptosis. Moreover, activation of the TrkA signaling cascades was suppressed by KK5101 treatment. Ex vivo tumor spheroid experiment disclosed that KK5101 significantly attenuated the expression of several mediators of TrkA signaling cascade, such as p-AKT, p-MEK, and p-STAT3, resulting in potent induction of apoptosis. Such results indicate that KK5101 may possess its antitumor effects by directly affecting cancer cell growth and/or survival via inhibition of TrkA signaling pathway. Overall, KK5101 is emerging as a promising therapeutic candidate for cancer treatment.

Poster Presentation : **MEDI.P-274**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Molecular dynamic simulation and Binding free energy estimation using Umbrella Sampling technique for Keap1-Nrf2 inhibitors

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Keap1-Nrf2 system is a biological defense mechanism in response to various stressors. An inhibitor of Keap1-Nrf2 interaction to activate Nrf2 expected as a novel target for drug discovery in oxidative stress-related disorders. Molecular dynamics with the explicit solvent has enormous potential for predicting protein ligand interactions. We have performed the Molecular dynamic studies to understand the protein-ligand behavior an alternative to simple docking procedure. Advance computational methods such as umbrella sampling, metadynamics, etc. provide rigorous and approximate methods for calculating absolute binding affinities for protein-ligand complexes. We have used four crystal structure 5FNU, 4XMB, 5CGJ, and 4L7B for Umbrella sampling study. Initially, MD simulation for 50ns performed using Gromacs Software. Principal component (PCA) analysis was employed to analyze the motion of flexible regions in the protein. 3D graphs for free energy landscapes generated, and structure corresponding to minimum energy basins was isolated. In US technique, Potential of mean force (PMF) graphs constructed for individual ligand by pulling it from binding site to bulk water. Obtained binding free energy values from PMF graphs were in line with the activity for individual ligands. Interaction energy between a ligand and 4Å surrounding residues during MD run calculated. Mechanistic details obtained from the MD simulation and US study have boosted our knowledge for the further development of novel and potent inhibitors for Keap1- Nrf2 cascade. We are also using pharmacophore-based virtual screening drug design approach for the development of novel inhibitors using Asinex, ChemDiv, life chemical, and FDA approved drug libraries.

Poster Presentation : **MEDI.P-275**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Development of Novel biased agonists against S1P1 receptor for Treatment of Multiple Sclerosis

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The sphingosine-1-phosphate receptors are the initial lipid G protein-coupled receptors that are divided into five subtypes; S1P1, S1P2, S1P3, S1P4, and S1P5. In particular, targeting S1P1 with the endogenous ligand, S1P, has shown substantial efficacy in treatment of multiple sclerosis (MS) since it promotes egress of lymphocytes from lymph nodes. The S1P receptor agonist has been shown to induce receptor down-regulation from the cell surface, suggesting that it acts as a functional antagonist of S1P1 to block lymphocyte egress by internalization of the receptor. In this study, we synthesized a series of derivatives and evaluated their biological activities and selectivity using a set of complementary assays such as Ca++ flux, β-arrestin recruitment, and S1P1 receptor internalization. Among the synthesized compounds, KDS1059 exhibited potent activities on β-arrestin recruitment and S1P1 receptor internalization with an EC50 of 182 nM and 12 nM, respectively, whereas it was slightly active (EC50=1720 nM) on Ca++ assay indicating that KDS1059 is a biased agonist. To optimize biased agonism, we synthesized KDS8000 series compounds by replacing the core part of KDS1059. Among the optimized compounds, KDS8024 exhibited most potent activities on β-arrestin recruitment and internalization with an EC50 of 0.23 nM and 0.05 nM, respectively. Peripheral lymphocyte count (PLC) assay was performed using blood samples from rats treated with KDS8000 series. KDS8007, KDS8022, KDS8024 reduced the number of peripheral lymphocyte which is similar effects to FTY720/fingolimod/Gilenya®. Furthermore, experimental autoimmune encephalitis(EAE) model experiments were conducted and KDS8024 effectively lowered the score of EAE mice. Taken together, KDS 8024 is most promising candidate with excellent biased agonism for treatment of MS.ReferencesBirker-Robaczewska, M. etc., al. Mol Pharmacol. 2018, 93, 109-118. Cohen, J. etc., al. Ann Neurol. 2011, 69, 759-777.Marsolais, D. etc., al. Nat Rev. 2009, 8, 297-307.

Poster Presentation : **MEDI.P-276**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Next Generation Antibody–Drug Conjugate(ADC) Technology; Evaluation of LCB’s Pyrrolobenzodiazepine(PBD)-ADC.

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Legochem Biosciences, Inc., Korea
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Antibody–Drug Conjugate(ADC) has become a promising alternative therapeutic approach for cancer patients since it enables targeted delivery of potent anti-cancer drugs to cancer cells. Today, four ADCs were approved and commercially available, along with nearly 200 ADCs under development. Here, we introduce LCB’s proprietary technologies of novel next-generation site-specific ADC platform technology, proprietary plasma-stable cleavable linker enabling cancer- specific release of payload, and proprietary Pyrrolobenzodiazepines(PBD) prodrug payload technology. Therefore, this presentation help you to understand the precise mode and mechanism of action of LCB’s proprietary technologies and their impact and influence on future development directions and clinical applications of next-generation ADCs.

Poster Presentation : **MEDI.P-277**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

YPN005, an oral CDK7 inhibitor, exhibits a significant antitumor activity in Myc-driven cancers.

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CDK7 is an important regulator of both cell cycle progression and gene expression by phosphorylating cell cycle kinase (CDK1, CDK2, CDK4 and CDK6) and RNA polymerase II (RNAPII). Recent studies indicate that the inhibition of CDK7 is an attractive strategy for the treatment of cancer by down-regulation of c-Myc expression. Myc regulates the anti-tumor immune response through CD47 and PD-L1 and drives an immunosuppressive phenotype in cancer. There are no existing therapies targeting Myc, which is highly prevalent in many difficult to treat cancers. We have investigated the therapeutic efficacy of YPN005, a novel oral CDK7 inhibitor, in triple negative breast cancer (TNBC) and hepatocellular carcinoma (HCC).The therapeutic efficacy of YPN005 was evaluated in TNBC xenograft mouse model. YPN005 was orally administered at a dose of 10mpk once a day for 3 weeks. THZ-1 which is reference compound was intravenously administered at a dose of 10mpk twice a day following the same schedule. We have observed tumor volume regression without any signs of toxicity during treatment periods.

Poster Presentation : **MEDI.P-278**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Identification of Target Protein of Novel Antifungal Agents Using an Affinity Bait and Chemical Reporter Strategy

Ji Won Choi, Bo Ko Jang, Siwon Kim, Hyeon Jeong Kim, Sun Jun Park, Jong Seok Yoo, AReum Song, Byung Eun Kim, Yoowon Kim, Jong-Hyun Park, Ki Duk Park[*]

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Cryptococcus neoformans is an opportunistic fungal pathogen that causes pneumonia and meningitis mainly in immunocompromised people. Current antifungal drugs have failed treatment for a variety of reasons, including direct drug resistance to *C.neoformans*. Therefore, it is necessary to develop new antifungal agents and to identify the target proteins for them to reveal the mechanism. We previously developed a novel series of functionalized amino acid (FAA) library for antifungal compounds and derived **KDS1090** as a potent lead compound by antifungal susceptibility (minimal inhibitory concentration (MIC)) test against representative fungal pathogens (**KDS1090** MIC: *C.neoformans* = 4 μg/mL, *C.albicans* = 16 μg/mL, *C.glabrata* = 16 μg/mL). Furthermore, we optimized FAA to improve antifungal efficacy and drug-like properties. Among the optimized compounds, **KDS5098** was the most promising drug candidate with excellent antifungal efficacies (MIC: *C.neoformans* = 2 μg/mL, *C.albicans* = 4 μg/mL) and drug-like properties (microsomal stability (human): 90%, (mouse) 78% remaining after 30 min; CYP inhibition (1A2, 2C9, 2C19, 2D6): $IC_{50} > 10$ μM, (3A4; 56% inhibition at 10 μM); single dose toxicity (mice): $LD_{50} > 1,000$ mg/kg; PK: F=40%). In this study, we attempt to identify targets and pharmacological pathways of lead compounds through a useful strategy called an affinity bait and a chemical reporter (AB&CR). First, we developed AB&CR agents containing isothiocyanate and alkyne group to identify their targets. We began the identification study by treating the C.neoformans soluble lysate with AB&CR agents and then reacting the treated lysates with chemical probe under cycloaddition condition. Furthermore, we would like to demonstrate drug binding target proteins through the AB&CR strategy for identify drug protein binding partners

Poster Presentation : **MEDI.P-279**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of siderophore equipped antibiotic to penetrate cell wall of Gram negative bacteria.

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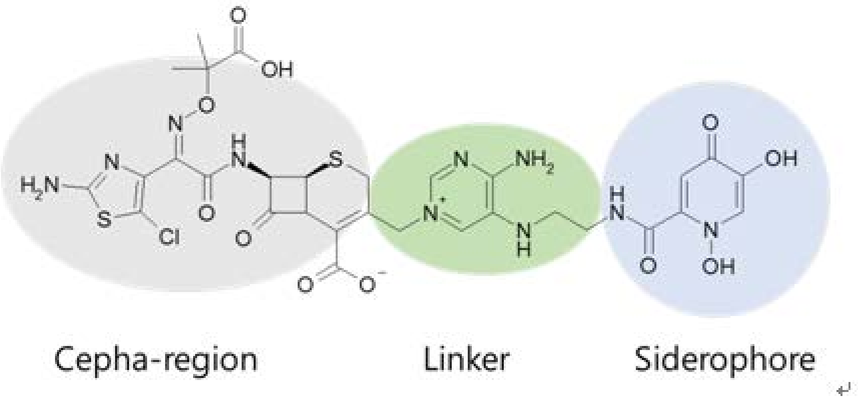
Legochem Biosciences, Inc., Korea

Nowadays, the Gram-negative bacteria research re-gained its interest due to the growing concern of the lack of treatment against drug-resistant bacteria. The mutations in outer membrane and porin channel are the main causes of this resistance, prohibiting the drug from penetrating into bacteria. To overcome these resistance, many research groups have mimicked "siderophore", high-affinity iron-chealating compound that bacteria produces to transport iron ion across cell membrane for its essential ingredient. Thus, siderophore was incorporated into the antibiotic via a specific linker to penetrate cell wall of bacteria, then its active ingredient would show antibacterial activity in the cell. LCB10-0200, was patented by LegoChemBioscience (US2012/264727) which represnts a typical example of this strategy in which cepha unit was connected to the dihydroxypyridinone siderophore via disubstituted pyrimidine linker. Here in this poster, we will show the total synthesis of LCB10-0200 in the original medicinal chemistry (mg scale) as well as the synthesis in view of process chemistry for larger scale (kg scale), specifically focused on the linker-siderophore unit.



Poster Presentation : **MEDI.P-280**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and Evaluation of Halogenated Vinyl Sulfones as Nrf2 Activators

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Parkinson's disease (PD) is a common neurodegenerative disorder that is characterized by abnormalities in motor control and muscle rigidity. Recent studies suggest that oxidative stress causes the striatal dopamine (DA) deficiency by neuronal loss in the substantia nigra (SN). The Nrf2 signaling is the main pathway responsible for cellular defense system against oxidative stress. Nrf2 is a transcription factor that regulates environmental stress response by inducing expression of various antioxidant enzyme genes. In previous work, we have synthesized novel vinyl sulfone derivatives as Nrf2 activator. The lead compound **KDS4048** was confirmed to activate Nrf2 and to induce expression of the Nrf2 dependent antioxidant enzymes such as HO-1, GCLM, GCLC, and NQO1 at both mRNA and protein levels in dopaminergic neuronal cells. In this work, we have optimized the lead compound **KDS4048** (EC_{50}=530 nM) to increase potency of Nrf2 activation. Compounds containing halogens and pyridine moieties into the vinyl sulfones were synthesized. Then, we compared potency and drug-like properties between the synthesized vinyl sulfone derivatives isomers. Among the synthesized compounds, **KDS4105** exhibited potent effect on Nrf2 activation (**KDS4105** EC_{50}=26 nM) in cell-based assay. We also confirmed its ability to induce the expression of anti-oxidant response genes HO-1, GCLM, GCLC, and NQO1 at both mRNA and protein levels and attenuate the PD-like motor dysfunctions in the MPTP-induced mice model of PD.

Poster Presentation : **MEDI.P-281**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Design, synthesis, and anti-inflammatory evaluation of hydrogen sulfide donor-peptide hybrids

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[1]*Chemical Advanced Materials, Gangneung-Wonju National University, Korea*

In recent years, hydrogen sulfide (H_2S) has been known as a critical signaling molecule that regulates many physiological and/or pathological processes. Emerging evidence of its therapeutic value is that this endogenous gaseous substance can modulate inflammatory processes. Indeed, H_2S donors have been shown to reduce edema formation and to inhibit pro-inflammatory cytokine synthesis. With the multiple biological actions of H_2S, there is a growing interest in developing various H_2S-releasing compounds for precise delivery of the gas to target tissues. Recently, combining nonsteroidal anti-inflammatory drugs (NSAIDs) with H_2S-delivery components have been shown to exhibit improved efficacy and reduced toxicity. In our group, hydrogen sulfide (H_2S)-releasing dithiolethione (ADT) functionalized with biologically active peptides has been investigated for their integrated anti-inflammatory and antioxidant potential. Series of ADT-peptides were synthesized and their inhibitory effects on LPS-induced inflammation in RAW264.7 cells were evaluated. Herein, our results demonstrate that the combination of H_2S donors with biological peptides have more potent effects. It would lead to promising anti-inflammatory agents for the treatment of peripheral and central inflammation.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **MEDI.P-282**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Conjugated Polymer-based Fibrillar Hydrogel for Artificial Extracellular Matrix

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Conductive polymers based hydrogel have gained immense interest due to its wide range of applications in tissue engineering and biomedical applications, including an extracellular matrix for tissue growth and regeneration, electrode for patient monitoring and electrotherapy, or as biosensors, and implantable bioelectronics. Owing to three-dimensional (3-D) porous structure, hydrophilic characteristics, and tunable chemical and physical properties, electroconductive hydrogel mimics the extracellular matrix in tissues and considered as a good matrix for cell growth, proliferation, and migration. Proceeding towards fabrication, electroconductive hydrogels are often dealing with low biocompatibility, high cytotoxicity, injectability, and adhesiveness. Herein, the electroconductive fibrillar hydrogel was prepared from chemically crosslinked electrospun nanofiber-based on polyvinyl alcohol (PVA) and with different poly(3, 4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) ratio. Physical, electrochemical, mechanical properties and biocompatibility were investigated to explore the impact of different amount of PEDOT: PSS loading. Chemical crosslinking between the hydroxyl group of PVA and sulfonic acid of PSS was confirmed by FTIR and swelling ratio. Also, the excess PSS to be considered as cytotoxic were removed during post-treatment, and confirmed by UV-Visible measurement. In addition, the 3-D neuronal culture of hippocampal neuronal cells on electroconductive fibrillar hydrogel with varying PEDOT: PSS loading showed the high viability and migration until 06 division. These results confer the feasibility of this scaffold to be used as extracellular matrix for neuronal tissue regeneration.

Poster Presentation : **MEDI.P-283**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Structural analysis and substrate synthesis of peptidoglycan peptidase3, a metallopeptidase that control the shape of helical cell

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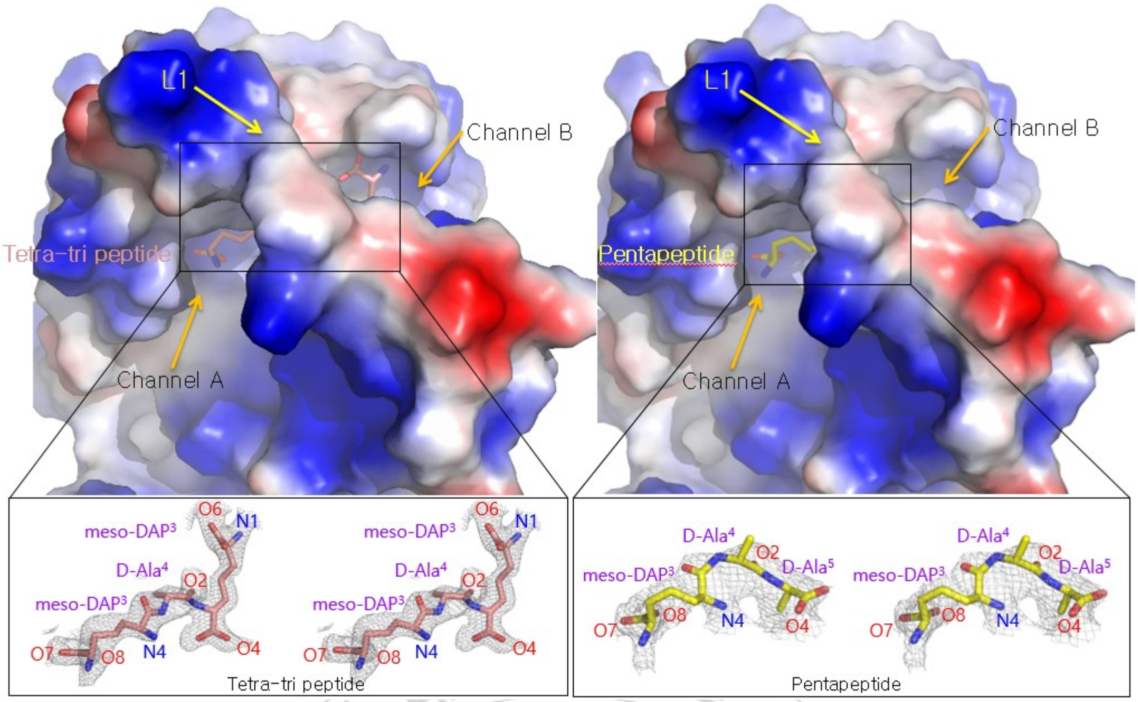
Helicobacter pylori and Campylobacter jejuni, which are known to be helical shaped Gram-negative bacteria, colonize the human mucus layer of the gastrointestinal tract and cause various gastrointestinal diseases such as chronic gastritis, peptic ulcer, gastroenteritis and gastric adenocarcinoma in humans.1,2 In the pathogenesis and gut colonization, the helical shape of H. pylori and C. jejuni is believed to be a very important factor in their motility improvement.3 Recently, a series of genes associated with maintaining the helical cell shape in these bacteria have been identified, most of which have been found to encode for either endo- or exoproteases that act on the peptide chains of peptidoglycan.4 These proteases are referred to as cell shape determining (Csd) proteins or peptidoglycan peptides (Pgp). According to recent studies, inhibition of proteins responsible for the helical cell morphology could be useful in interference with the bacterial virulence and lifestyle, hence a very attractive therapeutic target.5 However, their catalytic processes and substrate recognition are largely unknown. In this study, we describe the synthesis of two substrates for Pgp3, one of the Csd proteins, and the analysis of the Pgp3-substrate complex structures of the active site of Pgp3 in high resolution.


L1
Channel B
Tetra-tri peptide
Channel A
L1
Channel B
Pentapeptide
Channel A
meso-DAP^3
O6
N1
D-Ala^4
O2
meso-DAP^3
O7
O8
N4
O4
meso-DAP^3
O6
N1
D-Ala^4
O2
meso-DAP^3
O7
O8
N4
O4
Tetra-tri peptide
D-Ala^4
O2
D-Ala^5
meso-DAP^3
O7
O8
N4
O4
D-Ala^4
O2
D-Ala^5
meso-DAP^3
O7
O8
N4
O4
Pentapeptide

Poster Presentation : **MEDI.P-284**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Leucine-Rich Repeat Kinase 2 (LRRK2) small molecular inhibitors for Parkinson's disease (PD)

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Parkinson's disease (PD) is a neurodegenerative disease having motor symptoms such as tremor, muscular rigidity, shuffling gait, stoop posture, and slowing of movement. Leucine-rich repeat kinase 2 (LRRK2) protein mutations have been reported a leading cause of Parkinson's disease (PD). LRRK2 is a large (2,527 amino acids) multidomain with five putative domains and has composed of seven variants (LRRK2[G2019S], LRRK2[I2020T], LRRK2[S1761R], LRRK2[Y1699C], LRRK2[R1441C/G], and LRRK2[N1437H]) associated with the disease. Herein we will discuss the reported biological and chemical efforts for LRRK2 regulation. Since brain cells develop the disease, we looking forward to finding brain penetrant, highly potent and selective LRRK2 small molecules.

Poster Presentation : **MEDI.P-285**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Construction of Thiazole Derivatives using Liquid-Phase Synthesis

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Department of Pharmacy, Kyungpook National University, Korea

Liquid-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 Liquid-phase synthesis can be used usefully. Through this method, we have studied about the construction of heterocyclic compounds because heterocyclic compounds serve as key structural component of bioactive molecules. In this study, we have an interested in heterocyclic compounds containing thiazole moiety. we tried to construct a small molecule library based on thiazole moiety. Thiazole itselfs is not useful, but its derivatives are effective against dyes, sulphas, vitamin B (thiamin), fungicides, blood vessel blockers, analgesics, antiviral hypertension. For decades, humanity has been trying to reduce the side effects of many drugs. Therefore, we have developing a synthetic protocol to efficiently produce thiazole derivatives and generate a thiazole derivative library.

Poster Presentation : **MEDI.P-286**
Medicinal Chemistry
Exhibition Hall 1, THU 11:00~12:30

Construction of Chemical Library and Preparation of Drug-like Thiazole Derivatives using Solid-Phase Synthesis

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Kyungpook National University, Korea
[1]*college of pharmacy, Kyungpook National University, Korea*
[2]*Department of Pharmacy, Kyungpook National University, Korea*

Combination chemistry plays an important role in drug development because it is effective in building libraries of large amounts of compounds. In this study, we used a solid-phase synthesis method of combinatorial chemistry to build a library of ring-type thiazole derivatives among heterocyclic compounds that are biologically active and to find drug-like compounds.Thiazoles are five-membered ring heterocycles and their derivatives are considered a pharmacologically significant active scaffold that has almost all types of pharmacological activities.Their presence in peptides, their ability to bind to proteins, DNA, and RNA, as well as the exceptional range of antibacterial, antifungal, anti-inflammatory, anthelmintic, sedative, hypnotic, and antiretroviral properties of thiazole-containing compounds have directed numerous synthetic studies and new applications. Additionally, thiazoles are important features of various peptides and pseudopeptides that function as potent antineoplastic agents, or have demonstrated significant cytotoxicity or antibiotic properties.Owing to these interesting activities, we will build a large library through solid phase synthesis, which can produce a thiazole structure similar to other drugs.They are expected to have important biological activity and consequentially the production of large numbers of derivative libraries are likely to increase the possibility of drug development and supposed a significant role in the pharmaceutical industry.

Poster Presentation : **MAT.P-287**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Air cleaner miniature equipped with movable air filters for fast and efficient removal of PMs

Yoseph Lee, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

In recent years, particulate matter (PM) pollution has become a serious political, scientific, and public concern in many developing countries due to its significant impact on the living environments and public health. A lottery draw machine-inspired novel movable air filter (MAF) system is presented in which MAFs are vigorously moved or rotated to generate a high electric field and capture particulate matter (PM) particles. The MAF system purified 500 mL of a hazardous level of PM particles (2016 mg m-3 PM10 and 1040 mg m-3 PM2.5) at a high flow rate of 2.5 m s-1 with high removal efficiencies (99.7% and 98.8% for PM10 and PM2.5, respectively) in 1 min. The MAF system also had a small pressure drop of 3–6 Pa, which was approximately an order or orders of magnitude lower than previously reported values, even at a high flow rate of an order of magnitude higher than previously reported values. The MAF system exhibited excellent recyclability of up to 300 cycles with high removal efficiencies (99.7–98% and 98.8–96.2% for PM10 and PM2.5, respectively). Furthermore, the MAF system could effectively remove 500 mL of PM particles at extremely high concentrations (over 10 000 mg m-3 PM10 and over 3000 mg m-3 PM2.5) with very high efficiencies (over 99.8% and 99.6%, respectively) and a very low pressure drop (6 Pa), and these properties led to the conversion to clean ambient air (24 mg m-3 PM10 and 12 mg m-3 PM2.5) in 15 min.

Poster Presentation : **MAT.P-288**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Multifunctional Magnetic Sponge Ball for Environmental Remediation

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[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Oil spill accidents and industrial oily wastewater have become a severe environmental threat. Oil/water mixtures produced from industrial activities have been regarded as a serious issue because the discharge of oil/water mixtures has significantly increased due to increased industrial activity. Various materials and systems have been extensively developed for oil/water separation. Because oil/water mixtures produced from industries occasionally contain toxic organic compounds and heavy metals, there is an increasing demand for simultaneous oil/water separation and pollutant remediation. We report a multifunctional magnetic sponge ball for oil/water separation and pollutant purification. This sponge ball loaded with catalysts can decompose toxic organic pollutants in water while passing through the sponge ball. Furthermore, the sponge ball is able to selectively separate both water and oil from oil/water mixture by manipulation of an external magnetic field.

Poster Presentation : **MAT.P-289**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Magnetic sponge absorbent for cleanup of highly hazardous aqueous solutions

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[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

There is significant interest in developing novel absorbents for hazardous material cleanup. Hazardous materials, including strong acid/bases, oils, and solvents, are widely used in manufacturing industries in general. Spillages of these hazardous materials have devastating consequences for both human health and the environment. Thus, industries have made efforts to appropriately treat hazardous materials after use. Many approaches for hazardous material cleanup have been proposed, including neutralization, dilution, washing, bioremediation, solidification, or absorption. However, most previous studies have focused on synthesizing hydrophobic absorbents to remove oils and organic solvents. Relatively little attention has been paid to hydrophilic absorbents that can remove aqueous hazardous materials. We report an iron oxide/sponge absorbent that can naturally absorb a strong acid/base solution without an additional external force/absorption delay/overflow, generate fewer dust particles than the level of a clean room (class 100), and prevent the formation of droplet fragments during solution drop tests.

Poster Presentation : **MAT.P-290**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication of Conductive Fibers through Dip-Coating Surface-Modified AgNWs on Nylon Fibers

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[1]*Department of Chemistry, Kongju National University, 182 Shinkwan-dong, Kongju-si, Chungnam, 314-701, Korea*

Conductive fibers have attracted great research interest due to its potential applications on the area of suppressing static electricity, blocking electromagnetic waves and heating fabrics. Usually conductive fibers are made by electroless plating of conductive materials such as silver or copper on the surface of synthetic fibers such as Nylon. However, the conductive metal layers on the fibers are weak to external shocks and cracks may occur when the fibers were bending, drawing, making the conductivity decrease gradually during the daily life use. In this work, AgNW was coated on Nylon fibers as conductive materials, because of its high conductivity, flexibility and high aspect ratio. However the coating layers on the hydrophobic Nylon fiber were not uniform due to the hydrophilic polyvinylpyrrolidone surfactant of AgNW. Therefore, TA-mPEG was used as surface modification agent to remove the residual PVP of AgNW. The surface modified AgNW could be dispersed in some organic solvents and coated well on the hydrophobic Nylon fibers. The resistance was much lower than that of AgNW before the modification, and the coating efficiency was increased.

Poster Presentation : **MAT.P-291**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication of Bi-Containing Sea Urchin-like Pt Nanoparticles and Their Enhanced Electrocatalytic Properties for Methanol Oxidation

Kang Yeol Lee

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A facile method to synthesize Bi-containing sea urchin-like Pt nanoparticles is demonstrated. Bi-containing Pt particles were successfully prepared at 140 °C under atmospheric conditions. The atomic ratio of Bi to Pt was estimated by quantitative elemental analysis from the EDX data. A small amount of Bi (less than 10%) can induce the formation of sea urchin-like Pt nanoparticles. The presence of a small amount of Bi on the Pt surface had great impact on the catalytic performance of the Pt catalysts in methanol oxidation. Electrochemical studies of the methanol oxidation in an acidic medium using the Bi-containing sea urchin-like Pt nanoparticles were performed. The prepared nanoparticles exhibited enhanced electrocatalytic activity for methanol oxidation with a seven-fold higher oxidation current density and a more negative onset potential than commercial Pt/C (Pt 20%). Moreover, the current density of the Bi-containing sea urchin-like Pt nanoparticle/C catalysts was high even after 900 s of continuous electrocatalysis at 0.56 V. The synthesized Bi-containing sea urchin-like Pt nanoparticles should find attractive applications in various fields, such as fuel cells, sensors, and eletro- or organic catalysis.

Poster Presentation : **MAT.P-292**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Intimately Coupled Plasmonic Metal-Semiconductor-Graphene Ternary Heteronanostructures for Red-Light Responsive Photocatalysis

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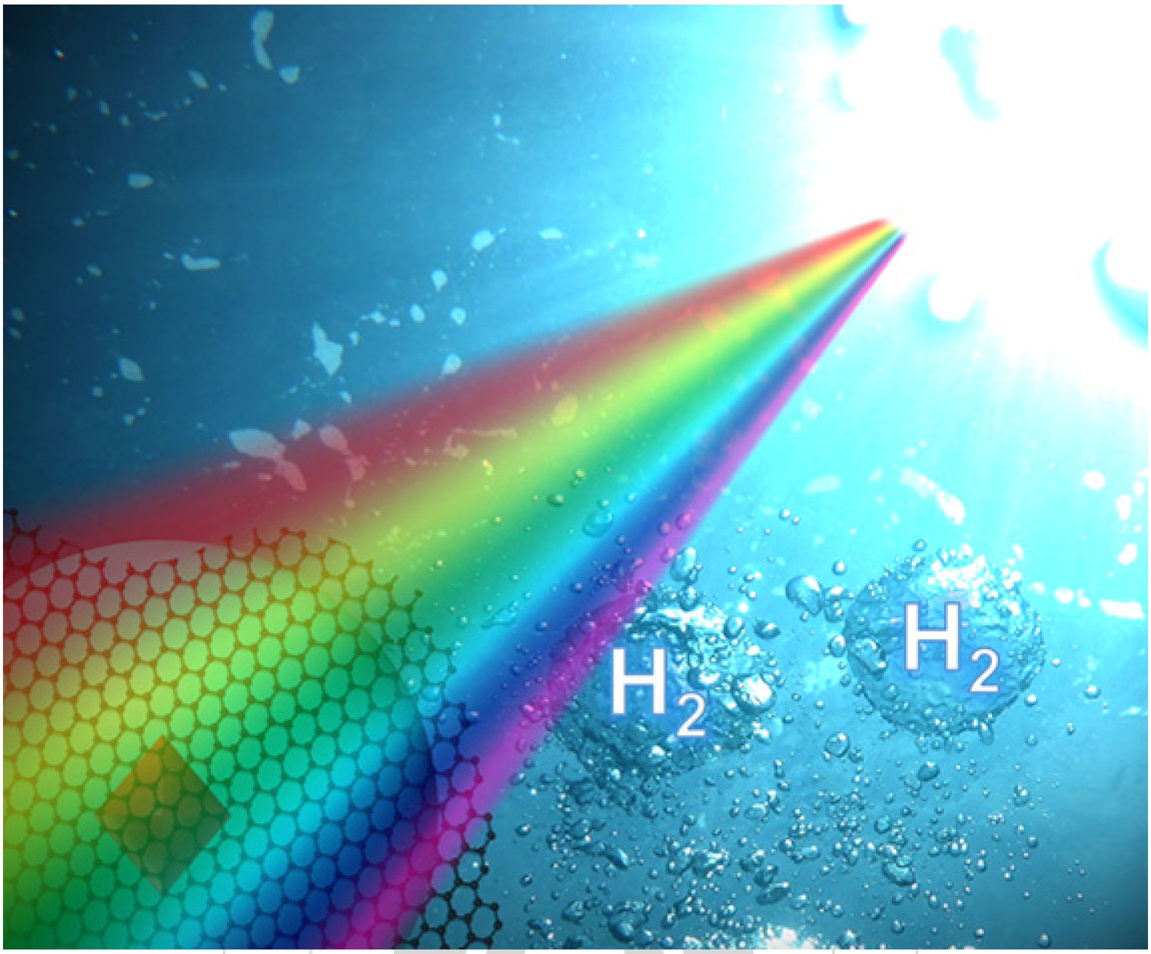
Design of heteronanostructures with controlled topologies and configurations is receiving ever-increasing attention to develop practical photocatalytic and photoelectrochemical systems. Herein, we present a promising solar energy conversion platform constructed by the intimate contact of plasmonic metal (octahedral Au nanocrystals), semiconductor (TiO_2), and graphene with a well-defined configuration. The shell engineering of Au nanocrystals with TiO_2 and graphene through sequential sol-gel, self-assembly, and post-calcination processes could allow the generation of graphene-encapsulated (octahedral Au nanocrystal)@(anatase TiO_2) core-shell nanostructures. The prepared ternary heteronanostructures exhibited superior photocatalytic hydrogen evolution activity over their binary counterparts, single-component catalysts, and physical mixtures of the constituents under visible-light irradiation ($\lambda > 400$ nm). Furthermore, they effectively utilized red-light region for photocatalytic reactions. Detailed mechanism studies on the photocatalysis revealed that the prominent photocatalytic performance of the heteronanostructures can be attributed to the transfer of plasmon-induced hot electrons from Au nanocrystals to TiO_2 and the subsequent migration of photogenerated electrons to graphene, which could be facilitated by the intimate contact between the constituent materials. This study can provide a new insight in devising heteronanostructures for efficient light harvesting.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Poster Presentation : **MAT.P-293**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

AgBiS2 Colloidal Nanocrystal Inks Prepared Using Solution-Phase Ligand Exchange for Solar Cell Applications

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Colloidal semiconductor nanocrystal inks have been attracted considerable attention for efficient thin film solar cells because of better surface passivation, ease of device fabrication, and room temperature solution-process. Herein, we demonstrate that highly-concentrated AgBiS2 colloidal nanocrystal inks dispersed in polar solvent can be prepared via solution-phase ligand exchange process using halometallates as a short inorganic ligand based on silver iodide (AgI) and bismuth iodide (BiI3). Considering that Ag-rich surfaces are dominantly exposed on AgBiS2 colloidal nanocrystals, we found that AgI-based halometallates anions (i.e., [AgI2]–) act as a main ligand for successful solution-phase ligand exchange. We also confirmed by ultraviolet photoelectron spectroscopy (UPS) the energy level tuning of AgBiS2 colloidal nanocrystals using various organic/inorganic ligands with different functional groups such as thiol, amine, halide, and carboxylate. Based on our results, we fabricated AgBiS2 nanocrystal solar cells, composed of AgI-based inks and ethanedithiol (EDT)-exchanged AgBiS2 nanocrystals, with improved open-circuit voltage (VOC) of 0.54 V resulting from better surface passivation and higher depleted width, compared to previous approach of AgBiS2 nanocrystal solar cells based on solid-state ligand exchange using only iodide-including ligands.

Poster Presentation : **MAT.P-294**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Highly Sensitive, Flexible and Transparent Polymer Thermistors Based on Silver Fractal Dendrites and Polyacrylate

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Polymer positive temperature coefficient (PTC) thermistors is attracting attention as temperature monitoring applications because they have several advantages including flexibility, conformability and biocompatibility. However, most polymer thermistors still have issues such as low sensitivity, low transparency, and poor operational durability because conventional conductive fillers have low electrical conductivity and inefficient hopping transport. Here, a highly sensitive and transparent polymer thermistor using silver fractal dendrites (AgFDs) and a polyacrylate has been demonstrated. It exhibits a superior PTC intensity (~10^7) around body temperature because of the high electrical conductivity of the AgFDs and the quantum tunneling effect resulting from their unique structures. Moreover, it exhibits excellent optical transparency, mechanical flexibility, and operational durability. In addition, electrical impedance spectroscopy analysis proved that the quantum tunneling effect amplified by the AgFD branch has a significant effect on the changes in resistance. Based on these characteristics, the thermistor was successfully demonstrated for real-time temperature monitoring of human body.

Poster Presentation : **MAT.P-295**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Preparation of Self-Healable and durable Superhydrophobic Film under facile UV Process at Room Temperature with Self-assembled Nanoparticles

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Inspired by the superhydrophobic lotus surface in nature, superhydrophobic functions with high water contact angle and small sliding angle, has attracted a lot of attention in industry. In this experiment, we can get superhydrophobic film with Durability and Self-Healing Ability by spray coating process at room temperature(RT). We synthesized a material with V-POSS and octadecanethiol under UV radiation at RT. The vinyl, functional groups, was substituted with octadecanethiol by thiol-ene click reaction, which has lower surface tension energy thanks to long alkyl chain. And to increase the roughness, we obtained self-assembled Al2O3 Nanoparticles with octadecyltriphosphonicacid(ODPA) which contributes to lower surface energy. After spray coating with made materials, the coated film results in a water contact angle greater than 150° and sliding angle smaller than 10°. And the film showed the superhydrophobicity even after both physical and chemical damages. The presented method can be used to various substrates like silicon, glass, even on flexible substrate like cotton.

Poster Presentation : **MAT.P-296**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Sensitive Detection of the Target molecular by Biosensor using Electrolyte-gate Thin-Film Transistor

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Printable and flexible thin-film transistors (TFTs) have gained significant attention over the last few years thanks to their implementation in many different sectors. Beside applications in large-area electronics such as flat displays, sensors and radio frequency identification tags, these devices have been widely investigated for life sciences applications too, including label-free biosensors, systems for drug delivery and implantable platforms. In this study, for low leakage and constant properties, we had demonstrated effective passivation via thiol-ene click reaction. This device is fabricated via UV curing and had a lower gate leakage current density than a device via SAM(Self Assembled Monolayer) method (1-Octadecanethiol). This device fabricated with 1,10-decanedithiol, Vinyl-POSS, Octadecanethiol. Also, these devices function well in repeated experiments. Additionally, this study presents a novel approach based on electoylte-gate thin-film transistor for the detection of tau protein one of the possible markers for the prediction of Alzheimer's disease (AD). The biosensor is based on the formation for stable aptamer-complexes on In2O3 surface covered with a layer of a self-assembled monolayer.

Poster Presentation : **MAT.P-297**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Hydrogenation of Nitroarenes by Pd-decorated GQDs

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Graphene quantum dot-based nanomaterials (GQDs) have received considerable attention as catalysts support in both photocatalysis and electrocatalysis. Some researchers have reported graphene-based metal nanocomposites show exhibiting good catalytic behaviour under various chemical reactions. However, the use of GQD-based nanocomposites in photocatalysis is rarely reported, perhaps because of the problem of dispersion and adhesion of nanoparticles onto GQD supports. In this regard, we synthesized a simple and effective method to prepare Pd-decorated GQDs by depositing Pd nanoparticles onto amine-functionalized GQDs. The prepared sample was characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Transmission electron microscopy (TEM), Raman spectra techniques. Pd-decorated GQDs exhibited an especially high catalytic activities for hydrogenation of nitroarenes.

Poster Presentation : **MAT.P-298**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Highly Efficient Perovskite Solar Cells via Additive Engineering

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One of the challenges of the scientific community working in green energy is to fabricate inexpensive and highly efficient solar cells to convert solar energy, the cleanest and most abundant renewable energy source available on Earth, into usable electrical energy. Recently, inorganic-organic hybrid perovskites as light harvesters have been considered as promising candidates for next generation solar cells. So far, a variety of efforts have been devoted to achieve a defect-less perovskite film with a high quality morphology for gaining a reduced loss-in-potential and an enhanced efficiency. In this work, we have prepared a high quality film of the mixed perovskite based on $(FAPbI_3)_{0.95}(MAPbBr_3)_{0.05}$ with a help of methylammonium chloride, which has a grain size of 300 ~ 1000 nm. Using the PTAA, the champion device showed a PCE of 21.6% with J_{sc} of 24.8 $mA \cdot cm^{-2}$, FF of 78.6 and V_{oc} of 1.10 (under reverse scan). The steady-state PCE corresponded to be a ~21.3%.

Poster Presentation : **MAT.P-299**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of Magnetite/Polystyrene Magnetic Composite Particle with Controllable Morphology

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Flower-like and core-shell magnetite/polystyrene colloidal composite particles have been prepared through a seeded dispersion polymerization with magnetite (Fe_3O_4) colloidal nanocrystal clusters (CNCs) as the seed, styrene (St) as the monomer. In addition silica (SiO_2) could be coated on the Fe_3O_4 CNCs to protect the magnetic nature of Fe_3O_4 CNCs from phase change. The morphology of the composite particles could be controlled by simply adjusting the weight ratio of the seed to the monomer (Fe_3O_4/St). The Fe_3O_4/PS colloidal composite particles showed magnetic behavior in an applied magnetic field. These different morphologies of the comosite particles may have great potential in biological/medical materials, sensors, catalyst, etc.

Poster Presentation : **MAT.P-300**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Promoting Activity and Selectivity of Electrochemical Chlorine Evolution Reaction by Atomically Dispersed Pt Catalysts

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Electrochemical chlorine evolution reaction (CER, 2 $Cl^-_{(aq)} \rightarrow Cl_{2(aq)} + 2\ e^-$) plays a pivotal role in both industrial and small-scale Cl_2 generation. Mixed metal oxides (MMOs) based on precious metals, such as Ru/Ir-based dimensionally stable anode (DSA), have been predominantly used as CER electrocatalysts. The MMOs are, however, also highly active for oxygen evolution reaction (OER), leading to the energy losses of electrolyzer systems and the degradation of MMO catalysts. Thus, the development of highly active and selective CER catalysts comprising minimal amounts of precious metals offers a pathway to reduce the Cl_2 production cost and its energy requirement. In this work, we demonstrate that an atomically dispersed $Pt{-}N_4$ sites on carbon nanotubes electrocatalyst (Pt_1/CNT) exhibits excellent CER performances in terms of overpotential, Tafel slope, turnover frequency, and stability, surpassing that of Pt nanoparticles on CNT catalyst (PtNP/CNT) and a commercial Ru/Ir-based DSA catalyst. Moreover, the CER selectivity of Pt_1/CNT was universally higher than that of DSA catalyst in the Cl^- concentration as low as 0.1 M and neutral pH. In situ X-ray absorption spectroscopy and density functional theory calculations suggest PtN_4C_{12} site as the most plausible active site structure. This work presents the first example of the atomically dispersed catalyst for the CER and is expected to provide an alternative for MMO catalysts.

Poster Presentation : **MAT.P-301**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Fabrication of Highly Conductive Nylon AgNWs/Fibroin Fiber Through Plasma Treatment

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Conductive fibers have received significant attention because of their possibility of use in wearable and foldable electronics. But the conventional conductive fibers that was fabricated by the electroless plating of Ag or Cu layers have weak strength and high cost of manufacturing. Silver nanowire (AgNW) and fibroin proteins were used to overcome the strength and high cost problems. AgNW have good conductivity and flexibility and Fibroin provide shield for Nylon fibers. However, it was difficult to combine AgNW solution with fibers because of AgNW solution's hydrophilicity and Nylon fibers' hydrophobicity. Plasma treated Nylon fibers were used in order to improve combination of AgNW and fibers. Plasma treated AgNW conductive fibers has higher more conductivity than untreated fibers. These AgNW conductive fibers could be used to wearable and foldable electronics.

Poster Presentation : **MAT.P-302**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Interfacial Property Dominates Thermopower of Molecular Junctions: Length Dependence of Seebeck Coefficient in Large-Area Junctions of *n*-Alkanethiolates

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Department of Chemistry, Korea University, Korea

Thermoelectric characterization of single molecules or monolayers could allow access to atomic-detailed structure-property relationship in organic thermoelectrics. Despite elegant and stimulating studies, the field of molecular thermoelectrics is still relatively unexplored as compared to molecular electronics. This presentation describes the length dependence of thermopower in self-assembled monolayers (SAMs) comprising structurally simple wide-bandgap molecules, n-alkanethiolates (SC_n; n = 2, 4, 6, 8, 10, 12, 14, 16, 18) chemisorbed on gold. Thermovoltage measurements at zero bias using liquid metal enabled the determination of the Seebeck coefficient of n-alkanethiolates for the first time. A plot of the Seebeck coefficient versus the length of the n-alkane chain reveals the presence of two different length-dependence regimes. The rate of decrease of the Seebeck coefficient as the molecular length increases changes at SC_{10} from −0.54 to −0.10 microV$(K\cdot n_C)^{-1}$. The theoretically proposed presence of metal-induced gap states (MIGS) in the short but not in the long n-alkanethiolates accounts for the two observed length-dependence regimes. Owing to the length dependence of the transmission function coefficient of MIGS in the short n-alkanethiolates, the Seebeck coefficient decreases linearly as the length increases. The nearly zero rate of decrease in the long n-alkanethiolates mirrors the insignificant MIGS in the long n-alkanethiolates. We envisage that the new energy states at the SAM−metal interface can be chemically tuned and harnessed for new applications in organic and molecular thermoelectrics and electronics.

Poster Presentation : **MAT.P-303**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Photodegradation of Rhodamine B based on TiO_2/Ag Nanoparticles supported on thiol-functionalized CNTs

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Titanium dioxide (TiO_2), due to its high efficiency, low toxicity, excellent physical and chemical stability, and low cost, has been one of the most widely investigated photocatalysts. However, the wide bandgap of TiO_2 (anatase: 3.2 eV and rutile: 3.0 eV) leads to a lower solar energy absorption, because TiO_2 is photocatalytically active under ultraviolet (UV) light. For this reason, many attempts have been made to synthesize new types of noble metal-mixed TiO_2 nanostructures (e.g., TiO_2/Ag, TiO_2/Au, TiO_2/Pt, etc.) for enhance photocatalytic activity and efficient use. In this study, we synthesized noble metal-mixed TiO_2/Ag decorated CNTs by introducing thiol groups on surface of CNTs. The samples were characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM). To study the photocatalytic activity, a 30 ppm of various dye solution was mixed with TiO_2/Ag decorated CNTs. Additionally, the photocatalytic activity was compared with those of a commercial P25 TiO_2.

Poster Presentation : **MAT.P-304**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

High Performance Plasmonic Perovskite Photodetectors with High Photocurrent and Low Dark Current Mediated by PEIE Buffer Layer Interfacial Engineering

Hannah Kwon, Dong Ha Kim*

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

Hybrid photodetectors based on organic-inorganic perovskites have witnessed rapid development due to their superior optoelectronic properties such as effective light absorption and high charge carrier mobility. Potential application of these materials has remained, however, limited due to high dark currents and low detectivity levels. In this work, uniformly synthesized Au nanorods (AuNRs) incorporated within a ~10 nm-thick polyethyleneimine ethoxylated (PEIE) interlayer were integrated into vertical perovskite photoconductive photodetectors. The localized surface plasmon resonance effects of AuNRs favored high photocurrent enhancement. Most notably however, the incorporation of a PEIE thin buffer interlayer served as a simple yet effective strategy to markedly suppress the dark current in these devices. The established synergetic effect between both components resulted in a significant enhancement of the device performance with high responsivity and detectivity. Our solution-processable plasmonic structures integrated within an interfacial polymer-based layer are simple, economic, and efficient for high-performance photodetectors.

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Poster Presentation : **MAT.P-305**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Non-hygroscopic F4-TCNQ doped TFB as Hole-Transporting Material forEfficient and Stable Perovskite Solar Cells

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The rational design of a hole transport material (HTM) is regarded as a key approach to improve the efficiency and stability of perovskite solar cells. Here, an efficient model is proposed by optimizing a conjugated polymer, TFB (Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(4,4′-(N-(4-sec-butylphenyl)diphenylamine)]), and a non-hygroscopic p-type dopant F4-TCNQ (2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane). F4-TCNQ-doped TFB serves as an ideal alternative to conventional HTM toward high hole mobility and suitable energy band alignment with perovskite material. The induced band alignment is proposed to be a primary factor to facilitate efficient charge extraction from the perovskite to the electrode and to increase the short-circuit current, which resulted in an enhanced power conversion efficiency of 17.46%. The hydrophobic nature of F4-TCNQ-doped TFB was shown to dramatically improve the long-term stability, maintaining ca. 80% of its initial efficiency after 10 days. Our simple, yet novel strategy paves the way for demonstrating a promising route for a wide range of highly efficient solar cells and photovoltaic applications.

Poster Presentation : **MAT.P-306**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Nonionic Biopolymer-Coated Upconversion Nanoparticles for the Highly Efficient Drug Delivery and NIR-Imaging

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A novel nanocarrier with great biocompatibility, imaging functionality, and drug delivery ability has been developed. In this work, the carrier poly(ethylene glycol)bis(amine)-modified alginate (Al-NH-PEG-NH_2) with folate (FA) as the targeting molecule (Al-NH-PEG-NH-FA) were synthesized to act as functionalizing agents for UCNPs. The synthesized polymer enhanced the stability, biocompatibility and upconversion luminescent intensity (20-fold) of the UCNPs compared to bare UCNPs. The UCNP-Al-NH-PEG-NH-FA nanocarrier enabled the specific targeting of folate receptor-positive KB cells, as confirmed via in *vitro* near-infrared (NIR) imaging. The anticancer drug doxorubicin (DOX) was loaded onto the nanocarrier with high drug loading efficacy (81.2%) then the pH-responsive drug releasing ability was measured. The release of DOX from the nanocarrier was pH-dependent, and the release rate was much faster at a lower pH (pH=5) than at a higher pH (pH=7.2). The in *vitro* evaluation of KB cells demonstrated that the DOX-loaded UCNP-Al-NH-PEG-NH-FA provided a sustained intracellular DOX release and a prolonged DOX accumulation in the nucleus, resulting in a prolonged therapeutic efficacy. Additionally, the DOX-loaded UCNP-Al-NH-PEG-NH-FA showed higher cytotoxicity towards the KB cells than free DOX. Thus, the biocompatible nonionic alginate-functionalized UCNPs hold the substantial potential to be further developed as effective NIR imaging agents and drug-delivery carriers.**KEYWORDS**: Nonionic; upconversion; doxorubicin; KB cells; nanocarrier

Poster Presentation : **MAT.P-307**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Detection on Catecholamines and cell imaging using $NaLuGdF_4$:Yb^{3+}/Er^{3+} upconversion nanoparticle

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The lanthanide based upconversion fluorescence material emits a photon of higher energy after the absorption of two low energy photons. The lanthanide based UC materials exhibit salient properties such as low harmfulness of low energy irradiation to analytes, high chemical stability, non-photobleaching, deep penetration, and non-autofluorescence interference. In this work, we present novel optical sensor and imaging agent for detection of catecholamines and cell imaging using $NaLuGdF_4$:Yb^{3+}/Er^{3+} upconversion nanoparticle (UCNP). The characterizations of the prepared materials were detailed. For sensing catecholamine, the different metals were decorated on UCNP materials to use as “triggers” for the specific detection. We found the optimum conditions for getting low limit of detections for catecholamines, dopamine, and epinephrine. Moreover, the prepared UC material exhibited as promising imaging agent for testing in vitro cell imaging on Hela cells. **Keywords:** imaging, sensing, upconversion

Poster Presentation : **MAT.P-308**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Study on Top-gate Top-contact Structure Thin-Film Transistor Based Bio-sensor Application

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Recently, There are various diseases in modern society. And some of diseases are difficult to treat after the onset. For example, Parkinson's disease, pancreatic cancer, Alzheimer's disease. However, some of these diseases produce biomarkers before the onset. so we have created bio-sensors that can detect these biomarkers.Top-gate Thin-Film Transistors (TFTs) Based bio-sensors, which have high sensitivity, low cost, low operation voltage easy fabrication and flexibility, and can be applied to mass production based on easy fabrication. Biosensors with these advantages are expected to be able to prevent and treat diseases easily in the future.

Poster Presentation : **MAT.P-309**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Well-dispersed Ni-/MnO-nanoparticle@porous carbon: highly reactive redox catalysts

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Bimetallic metal-organic framework-74s (MOF-74s) (Zn/Ni or Zn/Mn in various compositions), were synthesized, and Ni or MnO-doped carbonaceous materials were firstly prepared by direct carbonization of the MOF-74s under an inert environment for applying in redox catalysis. The obtained MOF-derived nanomaterials (MDNMs) were characterized thoroughly to understand their physicochemical properties including phase, porosity, particle size, dispersion, and composition. The porosity of the MDNMs increased but the size and content of Ni or MnO in the MDNMs decreased monotonously with increasing Zn content in the bimetallic MOF-74s. One MDNM(75Zn25Mn), prepared from MOF-74(75%Zn/25%Mn), showed noticeably higher activity in the oxidation of benzyl alcohol as compared with not only the MDNM(xZnyMn)s but also MnOx-loaded carbon or loaded γ-alumina (or, MDNM(75Zn25Mn) showed ~ 54 times turnover frequency (TOF) to that of MnO/activated carbon). MDNM(75Zn25Mn) was also effective in the oxidative removal of dibenzothiophene from a model fuel. Moreover, MDNM(75Zn25Ni), prepared from MOF-74(75%Zn25%Ni), had the highest TOF in the reduction of 4-nitrophenol among various MDNM(xZnyNi)s. The highest activity of MDNM(75Zn25Mn) and MDNM(75Zn25Ni), even with the lowest Mn and Ni contents in the respective MDNMs, for oxidation and reduction in several cycles might be due to the well-dispersed MnO (and Ni) and high porosity with mesopores. Therefore, it can be suggested that pyrolysised MOFs composed of mixed-metal can be utilized to get highly effective and reusable heterogeneous catalysts (with small sized and uniformly-dispersed active species) for various organic redox reactions.

Poster Presentation : **MAT.P-310**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Adsorptive removal of a wide range of contaminants of emerging concern with MOF-74(Zn)-derived carbon

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Recently, carbons derived from metal-organic frameworks (CDMs) are found as effective materials for the adsorption of various emerging concerns (CECs) from water. In this study, we prepared a series of CDMs using a few Zn-based MOFs (e.g. bio-MOF-1, MAF-4, MAF-5, MAF-6, and MOF-74 to yield CDM-1, CDM-4, CDM-5, CDM-6, and CDM-74, respectively) via high-temperature carbonization. The obtained materials were characterized by using various techniques including XRD, N2-adsorption-desorption isotherms, FE-SEM, FE-TEM, Raman, XPS, elemental and Boehm titration analysis. The CDM-74 shows a broader range of mesoporosity than the other CDMs although the BET-surface areas of the CDMs are comparable. After the widespread characterization, the materials were used as adsorbents for the removal of a wide variety of CECs, such as phallic acid, diethyl phthalate, N, N-diethyl-3-methylbenzamide (DEET), chloroxylenol and oxybenzone. The CDM-74 was found as the most efficient adsorbent among the tested adsorbents for all the studied CECs which is also superior or highly competitive with the reported adsorbents so far. Adsorption of DEET was studied in details, considering the highest increment (~6 times) for the DEET adsorption over the CDM-74 compared to AC. A plausible mechanism was elucidated from the adsorption results of DEET at a wide pH ranges as well as the functional groups presents on the CDM-74 and DEET. The recyclability or regeneration of the CDM-74 for adsorption was confirmed.

Poster Presentation : **MAT.P-311**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

CO2 capture with polyaniline-loaded metal-organic framework MIL-101(Cr)

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A metal-organic framework (MOF), MIL-101(Cr), was modified by introduction of polyaniline (PANI) via ship in bottle strategy in order to utilize basic moieties of PANI in capturing CO2 effectively from flue gas. PANI@MIL-101(Cr), with suitable PANI concentration, showed highly increased adsorption capacity for CO2, especially at low pressure of 0.15 atm, even though the porosity of MIL-101(Cr) was decreased upon PANI loading. Moreover, the PANI@MIL-101(Cr) showed increased selectivity for CO2 (against N2), compared with pristine MIL-101(Cr); and stable reusability. The observed favorable adsorption of CO2 on the PANI@MIL-101(Cr) might be because of basic species on well-dispersed PANI on the MOF. In order to improve performances of porous materials (such as MOFs) for CO2 capture, modification with PANI might be one way.

Poster Presentation : **MAT.P-312**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

The delivery of POSS (polyhedral oligomeric silsesquioxanes)-porphyrin nanomaterials into cells for possible PDT application

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Successful PDT agents require sufficient drug loading capacity, non-toxicity and specific tumor targeting ability. We have designed and synthesized various POSS (polyhedral oligomeric silsesquioxanes)-porphyrin nanomaterials for possible PDT application. We can control the number of POSS units in the porphyrin moiety as well as the relative position of POSS unit to the porphyrin skeleton. Studies on their effective uptake into cells have been performed. We also performed the systemic toxicity evaluation of POSS (polyhedral oligomeric silsesquioxanes)-porphyrin nanomaterials. We have investigated the role of POSS materials to enhance the cellular uptake of various POSS (polyhedral oligomeric silsesquioxanes)-porphyrin nanomaterials. Fundamental physical and chemical characterizations have been performed.

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Poster Presentation : **MAT.P-313**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Development of low temperature operating catalyst for exhaust gas treatment by using Fe-oxide

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Emission of harmful gases (e.g., CO, NO_x, and C_xH_y) from combustion of fossil fuels has become an important environmental issue. Generally, noble metals supported by alumina are used as commercial catalyst for conversion of those harmful gases to less harmful ones (e.g., CO_2, H_2O, and N_2), but the main drawback is their lack of catalytic activity at low temperature (<150ºC) which can cause so called ‘cold start-up’ problem. Attempts were made to lower operation temperature by using gold nanoparticles or other transition metal oxide based materials, however, their poor thermal stability restrains the commercial applications since catalytic activity should be retained after exposure to high temperatures for the exhaust gas treatment. In the present work, we incorporated Fe-oxide on commercial Pt/Al_2O_3 by using a simple temperature regulated chemical vapor deposition. By only using bare Pt/Al_2O_3, less than 10% of CO conversion to CO_2 was possible at room temperature, but upon 0.34 wt% loading of Fe on Pt/Al_2O_3, 80% of the conversion could be demonstrated. This superior catalytic activity at low temperature could be retained under various atmospheric conditions. The origin of the enhanced catalytic activity at low temperature was thoroughly studied by means of TEM, XPS, XRD, TPD, and TPR. We suggest that our catalysts have potential for industrial application due to the straightforward manufacturing process as well as high and stable catalytic activity.

Poster Presentation : **MAT.P-314**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Fabrication and characterization of thermo-responsive film

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Lately, research and development of external stimuli-responsive film have been studied actively. External stimuli can be largely divided into physical and chemical stimuli. In physical stimuli, there are many kinds of stimuli such as pressure, temperature, strain, magnetism, etc. In case of temperature, visualization technology is very important because it is difficult to detect by eye. In this study, the real-time color-changing temperature-sensivite film was fabricated and the characteristics of the film were analyzed. The film was made by coating with temperature sensitive material on the substrate, and the temperature and color change response time of the film were measured and compared.

Poster Presentation : **MAT.P-315**
Material Chemistry
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High-performance anion-redox cathode in potassium ion batteries

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Recently, ‘anion-redox chemistry’ has regained strong attention in the LIB community, because it can nearly double the charge-storage capability of cathode materials (Li-rich layered compounds such as $Li_{1.2}Ni_{0.13}Mn_{0.54}Co_{0.13}O_2$ and $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$) and thus dramatically improve the energy density of LIBs. However, the cathode materials that contain a substantial amount of mobile ions (Li^+, Na^+, and K^+) in an as-made state and show reversible sulfide-redox during charge/discharge (C/D) are quite rare. Surprisingly, we could find only a single example investigated for sodium ion batteries. To the best of our knowledge, O3-$NaCrS_2$ seems to be the only compound that shows sulfide-redox ($2S^{2-} \leftrightarrow S_2^{2-}$). O3-$NaCrS_2$ exhibited no discernable changes in Cr oxidation states during C/D, in contrast to iso-structural $LiCrS_2$, and delivered a reversible capacity of ca. 100 $mAh{\cdot}g^{-1}$. In this work, we for the first time present $K_{0.78}Fe_{1.61}S_2$ as an anion-redox cathode material for KIBs. The reversible change in the oxidation state of sulfides at high potentials during C/D is evidenced via various analysis methods. These experimental results are further validated via theoretical calculations. The relatively high capacities, which are ascribed to a cumulative anionic ($2S^{2-} \leftrightarrow S_2^{2-}$) and cationic ($Fe^{2+} \leftrightarrow Fe^+$) redox, and excellent cyclability and high-rate performance are also presented. We hope that this work will provide a new route in developing high capacity cathodes for KIBs.

Poster Presentation : **MAT.P-316**
Material Chemistry
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Porous tin nanoparticles: As an anode material for Mg-ion battery

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The next-generation energy storage batteries based on earth-abundant elements are in demand. Magnesium-ion batteries (MIB's) can be an attractive alternative for grid-scale energy storage due to the abundance of Mg resources and its high theoretical volumetric capacity (3833mAh/cm^3) compared to lithium-ion battery [850mAh/cm^3 (Graphite anode)]. The dendrite free nature of Mg is amenable for assembling high voltage and high energy density batteries with suitable cathode materials, but the passivating behaviors of the Mg in carbonate type electrolytes make it irreversible. The MIB has a low anodic window due to the electrolytes incompatibility with magnesium metal. There is a tremendous demand of anode materials for MIB's, which has a similar potential, high coulombic efficiency, and with high stability electrolytes. Tin (Sn), Antimony (Sb), Bismuth (Bi) and its alloys are the alloying/ de-alloying type anode candidates for next-generation batteries. In this work, bulk Mg_2Sn was synthesized by melting magnesium and tin powder at 750° C. Further, the as-synthesized Mg_2Sn was chemically de-alloyed in prior to make porous tin nanoparticles (PNP-Sn). Spectroscopic characterizations were performed to confirm the purity, porosity, and size of as-made PNP-Sn, in that XRD revealed the formation of pure crystalline Sn, XPS confirmed the absence of other chemical elements which were used in chemical de-alloying process, and FE-SEM revealed the porosity as well as size of Sn nanoparticles (

Poster Presentation : **MAT.P-317**
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Methane Chlorination with Chlorine Molecules using Zeolite Catalysts: Effects of Si/Al Ratios and Framework Types

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Methane (CH_4) chlorination with chlorine molecule (Cl_2) can produce various chlorinated products via C-H bond activation in CH_4. This reaction can occur spontaneously with irradiation of UV light even in the absence of a catalyst, which follows a free radical-mediated chain reaction mechanism. Therefore, the various products can be formed with a statistical thermodynamic distribution. In this work, CH_4 chlorination is controlled by using HY and MFI zeolites with various Si/Al ratios under various reaction conditions in order to break the thermodynamic product distribution and thereby produce a desired mono-chlorinated product (i.e., CH_3Cl). The results demonstrated that the framework type of zeolite and its Si/Al ratio could control the CH_4 conversion, CH_3Cl selectivity, and hence CH_3Cl yield under various reaction conditions. In particular, systematic correlations between the catalyst properties and CH_3Cl yield were constructed. Unfortunately, all the zeolite catalysts suffered from framework dealumination by HCl produced during the reaction, which was more pronounced for the zeolites having a high aluminum content. However, the extra-framework aluminum leached from the zeolite framework remained in the zeolite catalysts actively catalyzed CH_4 chlorination. The details of CH_4 chlorination and the results are going to be addressed in this poster.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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CO_2 Hydrogenation Using Mesoporous Metal Oxide Spinels Having Basicity

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Conversion of CO_2 to other chemicals (e.g., CO, methanol, hydrocarbon) in the presence of molecular hydrogen gas has been attracting great attention to many scientists. In this work, such hydrogenative CO_2 conversion has been investigated using mesoporous spinel-type metal oxides as heterogeneous catalysts. Aluminum based spinel materials having different divalent metal components (i.e., $ZnAl_2O_4$, $CuAl_2O_4$, $CoAl_2O_4$, $MgAl_2O_4$) have been synthesized and characterized with various tools. One remarkable feature of these materials is that they have different basicity (amount and strength) depending on the type of divalent metal cations. Accordingly, the binding affinity of catalytic surfaces to the acidic CO_2 molecule is totally different and hence they show very different catalytic performances. The results demonstrate that the conversion of CO_2 is proportional to the surface basicity of metal oxide spinel. These materials show high selectivity to CO except for $CoAl_2O_4$. Especially, $CuAl_2O_4$ having the strongest basic property shows high conversion of CO_2 and selectivity of CO.

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A Study on Surface coating of DNAM(Dinitroamelide)

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DNAM(Dinitroamelide) is synthesized by 1 step of nitration from melamine. The advantages of DNAM are high performance, hugh density, and insensitivity to impact and friction. But DNAM has some disadcantages. It has low volume yield in synthesis and is difficult to recrystallize. Furthermore, DNAM can be easily hydrolyzed to cyanuric acid at high temperature and humidity. A study of the coating of DNAM was undertaken to prevent DNAM from being hydrolyzed by moisture in the air.

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Poster Presentation : **MAT.P-320**
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Synthesis of supported Pt NPs on TiO_2 toward oxygen reduction reaction

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The proton exchange membrane fuel cells (PEMFCs) and direct methanol fuel cells (DMFCs) are attention to environmentally friendly green energy and high density energy, for portable electronic devices, because they have high energy for simple system designs and low pollutant emissions. In particular, Pt-based nanomaterials are currently the most popular and efficient cathode materials used in fuel cell. Pt catalysts are widely used as electrocatalysts for oxygen reduction reaction (ORR) in fuel cells because of their unique ability to facilitate the catalytic reactions, but high price limit its wide use. To increase the activity and monodispersion of Pt catalysts, carbon support has been widely used as catalysts. Furthermore, carbon support has various advantages such as large surface area and low cost. However, Pt catalysts are still exposed to poisoning and causticity. This disadvantage would cause Pt agglomeration in the operation of the fuel cell, resulting in loss of activity catalyst and stability after electronic reaction. To solve this problem, the method of supporting a metal oxide on a Pt catalyst has attracted very interest. Supported Pt catalyst on metal oxide increase current activity and stability because metal oxide have strong metal support interaction toward supported Pt catalysts. In the present work, we synthesized a polyol system for the formation of TiO_2-Pt catalysts. The prepared TiO_2-Pt catalysts exhibited considerably improved electrocatalytic performance toward ORR compared to commercial Pt/C catalysts. We anticipate that the present approach will be helpful to develop efficient electro catalytic systems for practical applications.

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Thermalstability of new ion exchangers based on Acrylonitrile

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Using thermogravimetric method, the thermostability of new ion exchangers obtained by chemical modification of porous copolymer of acrylonitrile with divinylbenzene has been studied. The chemical modification of the crosslinked acrylonitrile-divinylbenzene copolymer is based on a polymer-analogous reaction converting the functional groups of the copolymer under the influence of alkali and various amines. Thermogravimetric studies show that the heating process of the new ion exchangers is accompanied with a variety of endothermic and exothermic effects. Decrease in mass in range of 150 – 180 °C was mainly related with disappearance of hygroscopic and crystallization water. The irreversible changes in the chemical structure of the polymers to form a cyclic structure and intermolecular bonds, as well as the allocation of certain amounts of H_2, NH_3, HCN, CO_2 were observed in range of 180-300°C. A further increase in temperature of the system was accompanied by increasing heat release due to thermo-oxidative degradation and rupture of C-C backbone. In particular, the total mass loss of anion exchangers AN:DVB:GG, AN:DVB:GA, and AN:DVB:DEA was not excess of 72 % at 500 °C. These results confirm the thermal resistance of new prepared ion exchangers. **Keywords:** ion exchanger, thermal stability, endothermic, exothermic effect, thermo-oxydation degradation.

Poster Presentation : **MAT.P-322**
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Hydrogen Evolution Reaction Kinetics of Pd@Pt Core-Shell Nanocrystals in Alkaline Electrolytes

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Because hydrogen (H_2) gas has received great interests owing to its utilization as an energy carrier and a fuel in electrochemical devices, its production via a hydrogen evolution reaction (HER) in acidic and alkaline electrolyzers has been intensively investigated for practical use. Therefore, the rational design of electrocatalysts based on HER mechanisms (Volmer-Heyrovsky-Tafel) has been proposed to optimize the strength of H adsorption (H_{ad}) on metallic catalyst. To assess this, we prepare Pd@Pt and PdH@Pt core-shell octahedra enclosed by Pt(111) facets as model catalysts for controlling the ΔG_H affected by ligand, strain, and their ensemble effects. The Pt shell thickness is adjusted from 1 to 5 atomic layers by varying the amount of Pt precursor added during synthesis. Our electrochemical results showed that the HER activity was slightly improved on Pd@Pt octahedra compared to that on PdH@Pt octahedra and was further improved by the increased number of Pt shell in an alkalin electrolyte. Interestingly, these experimental results do not accurately correspond with ΔG_H values calculated by the first-principles density functional theory. From the mismatches between the HER activity and ΔG_H values, we show that the alkaline HER does not simply follow the thermodynamic scaling relationship but is concurrently governed by kinetically-controlled reorganization of interface water molecules.

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Synthesis and Electrochemical Performance of π-Conjugated Molecule Bridged Silicon Quantum Dots Cluster as Anode Material for Lithium Ion Batteries

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π-Conjugated molecule-bridged silicon quantum dots (Si QDs) cluster was prepared by Sonogashira C-C cross-coupling reaction between 4-bromostyryl and octyl co-capped Si QDs (4-Bs/Oct Si QDs) and 1,4-diethynylbenzene. The surface chemical structure, morphology, and chemical composition of the Si QDs cluster were confirmed by Fourier transform infrared spectroscopy, field emission transmission electron microscopy, and energy dispersive X-ray spectroscopy. Lithium ion batteries were fabricated using the 4-Bs/Oct Si QDs and the Si QDs cluster as anode materials to investigate the effect of QDs clustering on the electrochemical performance. Compared with the 4-Bs/Oct Si QDs electrode, the Si QDs cluster electrode exhibits improved electrochemical performance, such as a high initial discharge capacity of ~ 1957 mAh·g^{-1} and good cycling stability with ~ 63 % capacity retention following 100 cycles at a current rate of 200 mA·g^{-1} when tested at the voltage window of 0.01~2.5 V. The improved electrochemical performance of the Si QDs cluster can be attributed to the π-conjugated molecules between the Si QDs and on surface of Si QDs cluster, which serve as a buffer layers to alleviate the mechanical stresses arising from the alloying reaction of Si with lithium and maintains the electrical conduits in anode system.

Poster Presentation : **MAT.P-324**
Material Chemistry
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Synthesis of CuIn(S,Se)2 thin films from molecular precursor solution for photovoltaic device

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Chalcopyrite absorber material for photovoltaic device is an interesting topic with some advantages such as high stability and high efficiency. The solution-processed method for the preparation of this material have been explored to achieve low cost and simple control of film homogeneity. Here, CuIn(S,Se)2 (CIS) thin films have been synthesized from molecular precursor solutions. N, N-dimethylformamide (DMF) and thiourea are used as a solvent and a ligand to coordinate copper and indium metals. The synthesized thin films with ~1.5μm thickness have tetragonal phase CuIn(S,Se)2 which was composed of In-rich large-grain top layer on molybdenum substrate. Crystal structures of the thin film have been determined by powder X-ray diffractometer and Raman spectrocopy. Modification of molecular system of Cu and In-thiourea was investigated SEM and EDX were utilized to analyze morphology of the surface and to study composition of absorber layer of CIS photovoltaic devices.

Poster Presentation : **MAT.P-325**

Material Chemistry

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Anion effect on growth of LiAl-layered hydroxides nanocrystal on aluminium metal substrates

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We synthesized an $LiAl_2$-layered double hydroxide(LDH) on an aluminum metal foils in an aqueous lithium salt (LiX, X = CO_3^{2-}, NO_3^-, Cl^-, SO_4^{2-} salts, respectively) solution by urea hydrolysis to adsorb lithium cations. This work presents a method for directly growing oriented $LiAl_2$-LDH nanocrystal on aluminum metal foils. Concentration of as-adsorbed lithium cations was associated with height of LDH layer on aluminum metal foils. The height of LDH layer synthesized with Li_2SO_4 has the largest value for single anion; CO_3^{2-}, NO_3^-, Cl^-, SO_4^{2-}. $LiAl_2$-LDH synthesized by mixed anion including SO_4^{2-} increased in height of LDH layers rather than sigle anion. Concentration of lithium cations in $LiAl_2$-LDH on aluminum metal foil was determined by inductively coupled plasma (ICP). Morphology and crystal structure of $LiAl_2$-LDH were confirmed by scanning electron microscopy (SEM), X-ray diffraction (XRD).

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Investigation of self-bias magnetoelectric responses in multiferroic polymer composites

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Magnetoelectric(ME) effect is defined as a response voltage given by an electrical polarization under applying a magnetic bias field(Hbias). The ME responses can be obtained with high reliability under very small magnetic field change of 1 nT. ME composites have attracted great interest for feasible applications such as energy harvesters, magnetic-/electric- sensors, and nano-actuators. Recently, polymer-ceramic ME composites have been developed with facile processing techniques and high flexibility to increase feasibility of ME devices. Further, typical ME responses can be obtained under a Hbias, which requires a bigger size electromagnet being a critical limitation for device application. So, several research groups have developed self-bias ME effect in ceramic-based composites to induce effective strain change in magnetostrictive phase without electromagnet since 2010.In this study, self-biased ME responses were investigated in polymer composite films of $BaTiO_3$@$CoFe_2O_4$-Ni/PVDF. First, two-phase $CoFe_2O_4$-Ni magnetostrictive structure was synthesized by hydrothermal process. The magnetostrictive structure was found to exhibit vertically standing $CoFe_2O_4$ nanosheets with a thickness of ~ 30 nm and a lateral size of ~ 800 nm connected on a porous Ni films with a film thickness of 1.6 mm and a pore size of 0.25 mm. Then $BaTiO_3$ was coated on the magnetostrictive structure via sol-gel synthesis to suppress leakage current during poling process as well as to enhance dipole moment for high piezoelectricity. Final structure of $BaTiO_3$@$CoFe_2O_4$-Ni/PVDF films was developed by infiltration of PVDF and then ME responses were investigated with impedance analysis under an off-resonance frequency of 1 kHz. In a result, a self-bias ME response was confirmed under zero DC magnetic field.

Poster Presentation : **MAT.P-327**
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Microwave-assisted synthesis of reduce graphene oxide with hollow nanostructure for advanced lithium storage application

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Reduced graphene oxide as an anode in lithium ion batteries has gathered much research interest due to its electrochemical stability and moderate energy density. Because the energy density of reduced graphene oxide is lower than that of metal and/or metal oxide electrode, incessant attempts have focused to enhance the discharge capacity of reduced graphene oxide. In this study, microwave-assisted synthesis of reduced graphene oxide with spherical hollow structure was successfully performed by using chemical interaction between building blocks. Electron microscopy images of the product showed that this reduced graphene oxide maintained its hollow nanostructure even after the template removal. The discharge capacity of the product was much larger than that of conventionally synthesized graphene, showing that the nanostructured framework of microwave-irradiated reduced graphene oxide could provide a large number of insertion sites easily accessible by lithium ions.

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Ge/GeO_2/graphene nanocomposites as anode materials for lithium ion batteries

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Germanium-based nanoparticles with theoretically high lithium storage properties have attracted much research interest as potential anode materials in lithium ion batteries. However, metal or metal oxide had inherent problems of long term performance in lithium storage applications because of their large capacity fading during charge/discharge cycles. In this study, the Ge/GeO_2/graphene composites were synthesized to overcome such demerits. Encapsulating germanium-based nanoparticles between matrices of reduced graphene oxides were expected to offset volume expansion effect. Transmission electron microscopy images revealed that Ge/GeO_2 nanoparticles were distributed onto the reduced graphene oxides. According to the electrochemical discharge/charge experiments, the discharge capacity of the bare Ge-based nanoparticles was decreased rapidly upon successive cycles, while the present composite had superior cycling stability.

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Hydrogen Production from Formic Acid Decomposition Using Pd−Ag Bimetallic Core−Shell Nanostructure

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To develop high-performance bimetallic catalysts, fine control over both the ligand and strain effects of secondary elements on the catalytic function of primary elements is crucial. Here we introduce an approach to produce Pd−Ag bimetallic core−shell nanocatalysts with synergistic regulation of the ligand and strain effects of Ag. Through precise core−shell engineering, (PdAg alloy core)@(ultrathin Pd shell) nanocrystals with controlled core compositions and shell thicknesses in addition to a well-defined octahedral morphology could be realized. The prepared octahedral PdAg@Pd core−shell nanocrystals exhibited pronounced catalytic performance toward hydrogen production from formic acid decomposition. The maximum catalytic activity was achieved with PdAg@Pd nanocrystals consisting of PdAg alloy cores with an average Pd/Ag atomic ratio of 3.5:1 and 1.1 atomic layer of Pd shells, which showed a record high turnover frequency of 21 500 h^{-1} at 50 °C. This catalytic function could be attributed to the optimized combination of the electronic promotion and lattice strain effects of Ag on Pd. We envision that the present work can provide a rational guideline for the design of improved catalysts for various important chemical and electrochemical reactions.

Poster Presentation : **MAT.P-330**
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Synthesis and Structural Characterization of New Cluster Quaternary Chromium Thiophosphates, A_2CrPS_6. (A=Rb, Cs)

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The new cluster quaternary chromium thiophosphates, A_2CrPS_6 (A=Rb, Cs) have been synthesized though reaction of the elements powder with ACl as a reactive flux at high temperature via solid state reactions. The crystal structures have been determined by single crystal X-ray diffraction techniques. The title compounds are built up from the cluster binuclear thiophosphate anion, $Cr_2P_2S_{12}{}^{2-}$, which is composed of a pair of edge sharing Cr-centered octahedron and P-centered tetrahedron. These cluster units and alkali metal cations, A^+ are bound through ionic interactions. The classical charge valence can be described as $[A^+]_2[Cr^{5+}][P^{5+}][S^{2-}]_6$. To the best of our knowledge, the title compounds are the first examples of the penta-valent Cr ion in sulfides.

Poster Presentation : **MAT.P-331**

Material Chemistry

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Synthesis and Structural Studies of a New Two-dimensional Quaternary Sulfide, $Cs_2HfPd_3S_6$

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The new quaternary sulfide, $Cs_2HfPd_3S_6$ has been synthesized from elemental powders through alkali metal halide flux methods and it is structurally characterized by single crystal X-ray diffraction techniques. The Hf atom is surrounded by six S atoms in a trigonal prismatic fashion. Two HfS_6 units are bridged by two Pd atoms by sharing edges to form the basic repeating units. These units are linked together to complete the infinite anionic two-dimensional layer, 2¦∞[$HfPd_3S_6^{2-}$]. These layers stack on top of each other and the Cs^+ ions reside between the layers to satisfy the charge neutrality. The charge valence of the title compound can be described as $[Cs^+]_2[Hf^{4+}][Pd^{2+}]_3[S^{2-}]_6$. In this presentation, a comparison of the title compound with the previously prepared related phases, $CsTaPd_3S_6$ and $K_2Ta_6Pd_9S_{24}$ will be discussed.

Poster Presentation : **MAT.P-332**
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Facile synthesis of PtNi alloy nanodendrites on CeO_2 nanosheets as supporting materials with fine electrocatalytic performances toward methanol oxidation and oxygen reduction reaction

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The development of supporting material for electrocatalysis with additional promoting effects is essential for designing innovative fuel cell catalysts. Due to its high density of oxygen vacancies, CeO_2 enables to suppress the poisoning of active sites in Pt-based catalysts and is considered to be one of the best candidates for supporting materials. Here, we report a facile one-pot synthesis strategy for $PtNi/CeO_2$ hybrid nanostructures with well-defined and dispersed dendritic PtNi nanocrystals on CeO_2 nanosheets as supporting material. The prepared $PtNi/CeO_2$ nanostructures exhibited outstanding electrocatalytic properties toward both methanol electro-oxidation and oxygen electro-reduction owing to high oxygen storage capacity of CeO_2 support and arbitrated electronic structure. CeO_2 nanosheets, the reinforced supporting material than other carbon based, enhanced not only the activity but also durability of the catalysts.

Poster Presentation : **MAT.P-333**
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Near-infrared phosphorescence emissive Iridium (III) complexes with substituent variation for solution processable red-NIR organic light-emitting diodes

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Research on near-infrared- emitting materials and devices has been studied for decades with fundamentaland practical application demands such as night-vision displays ,phototherapy and civilian medical diagnostics. However, the development of stable, highly efficient and low-cost NIR-emitting luminophores faces challenge due to the vulnerability of the small emissive bandgap toward several nonradiative decay pathways. Novel and distinct molecular designs are needed for yielding an intense NIR emission. Herein, we developed a series of deep-red to NIR emissive iridium(III) complexes (Ir1–Ir4) to analyze the effects of electron-donating and electronwithdrawing substituents anchored on the main ligands. These substituent variation induce the emission bandgap systematically from the deep-red to the NIR region while altering the emission efficiencies. Single-crystal X-ray structures authenticated the exact coordination geometry and intermolecular interactions in these new compounds. Photophysical study were also performed in the solution, neat powder, doped polymer film, and freeze matrix at 77 K states to investigate the effects of substitution on the excited-state properties. These studies were conducted in conjunction with density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations. Finally,the –CH_3 substituted Ir1, unsubstituted Ir2, and –CF_3 substituted complex (Ir4) were promising novelcompounds with bright phosphorescence quantum efficiency in doped polymer films. Using these novelmolecules, deep-red to NIR emissive organic light-emitting diodes (OLEDs) were fabricated and the unoptimized device exhibited maximum external quantum efficiency (EQE) values of 2.05% and 2.11% for Ir1 and Ir2, respectively.

Poster Presentation : **MAT.P-334**
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Virus-based Directed Growth of Ultralong Single-Crystal Silver Nanowires

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These days, electronic devices demand high performance electrode. Ag nanowire is the most promising candidate because it has excellent electrical property, however, the process of Ag nanowire synthesis is complicated and it is difficult to obtain long-scale single Ag nanowires in traditional methods.M13 bacteriophage is a helical structured biomaterial with 6.6 nm of the diameter and 880 nm of the length. M13 bacteriophage can be reproduced through self-cloning and modified the chemical properties by genetic engineering. According of these properties, M13 bacteriophage is very useful as a template. In this work, we fabricated ultra long-scale single Ag nanowire using genetically engineered M13 bacteriophage as a template. We observed that the crystallinity of Ag nanowire (length or diameter) was affected as changing the engineered chemical structure on major coat protein of M13-bacteriophage. The range of Ag nanowire was around 50 nm to 200 nm and the average length and diameter were around 100 um and 1 um, respectively. The maximum length of Ag nanowires that was observed was 600 um. The existence and morphology of Ag nanoparticles and nanowires were confirmed by FE-SEM (field emission scanning electron microscope) and high resolution TEM (transmission electron microscope). To examine the components of Ag nanoparticles and nanowires, map profiling was conducted by EDS (energy dispersive spectroscopy).

Poster Presentation : **MAT.P-335**
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Antimony Doped Layered Cathode Materials for Sodium Ion Batteries with Improved Cyclic Stability and Rate Performance

Dominic savio Muthu gnana theresa nathan, Myoungho Pyo*

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Sodium ion batteries (SIBs) have been receiving great attention from battery researchers as promising alternative to lithium ion battery (LIB) technology. Among various cathode materials, layered metal oxides gained significant interest due to high specific capacity and fast diffusion via 2D channel. In particular, O3-$NaCrO_2$ has been investigated as positive electrode for SIBs and it delivered specific capacity of 110-120 mAh g^{-1} with average working voltage of 3.0 V. However, O3-$NaCrO_2$ electrode suffers from rapid capacity fading and poor rate performance mainly attributed to phase transitions and electrolyte side reactions during the cycling process. In the present work, we made an attempt to prepare Sb doped layered materials ($Na_{1-2x}Cr_{1-x}Sb_xO_2$) by solid-state reaction. The doping of Sb could influence cation ordering between Cr^{3+} and Sb^{5+} resulting in improved electrochemical performance. By carefully tuning the doping content of Sb and reaction temperature, we obtained two different structures such as O3-$Na_{0.8}Cr_{0.9}Sb_{0.1}O_2$ and P2-$Na_{0.7}Cr_{0.85}Sb_{0.15}O_2$. When tested as cathode material for SIBs, the O3-$Na_{0.8}Cr_{0.9}Sb_{0.1}O_2$ electrode displayed a specific capacity of 110 mAh g^{-1} with average working voltage of 3.2 V. The enhanced average working voltage compared to bare O3-$NaCrO_2$ could be attributed to the inductive effect of Sb^{5+} ions. The P2-$Na_{0.7}Cr_{0.85}Sb_{0.15}O_2$ delivered a specific discharge capacity of 80 mAh g^{-1} at a current rate of 0.1C. It also demonstrated superior cyclic stability with 90% initial capacity retention after 300 cycles at 1C. The results show that the Sb doped layered cathodes as promising cathode materials for sodium ion batteries.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

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Poster Presentation : **MAT.P-336**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Ca-ion dual graphite battery utilizing ternary ionic liquid based electrolyte

Prabakar Richard, **Myoungho Pyo**[*]

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Considerable progress in divalent Mg^{2+} and Ca^{2+} ion batteries has stirred up renewed research interest in the past decade. However, the implementation of this technology to a large extent has been obstructed by the absence of a suitable electrolyte capable of simultaneously supporting reversible electrochemical reactions on the two electrochemical extreme potential limits i.e., above 4.5V and near 0 vs. Li. Calcium ion batteries (CIBs), in particular still suffer from electrolyte-incompatibility with metallic and graphite anodes. In our previous work, we reported graphite as a reliable Ca^{2+}-intercalation anode in tetraglyme (G_4),[1] however, the electrolyte was unable to operate at high voltage due to the thermodynamic tendency to decompose at potentials well below required for a reversible anion intercalation reaction to occur in a graphite cathode. Herein, we report that by formulating a ternary electrolyte by careful optimization of the relative Ca electrolyte salt concentration to a glyme solvent in combination with ionic liquids, the two electrochemical extreme potential limits were comfortably extended permitting reversible and stable electrochemical reactions in a dual graphite type cell. Successful intercalation of Ca^{2+} and $TFSI^-$ ions at the graphite anode and graphite cathode were witnessed, respectively. Investigations revealed that optimized concentrations promote complex aggregates formations effectively suppressing free-solvent decompositions at high voltages. This enabled us to construct a dual–graphite cell with good cyclic stability.Reference[1] S. J. Richard Prabakar, A. B. Ikhe, W. B. Park, K.-C. Chung, H. Park, K.-J. Kim, D. Ahn, J. S. Kwak, K.-S. Sohn, M. Pyo, *Adv. Sci*,. (under revision) 2019.

Poster Presentation : **MAT.P-337**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Preparation of red emitting Rb2KSiF7:Mn4+ phosphor for white light LED application

Kangsik Choi, Younbong Park*

Department of Chemistry, Chungnam National University, Korea

Recently, phosphors activated with non-rare earth metals which are relatively inexpensive than rare earth metals activators have been in the spotlight. A K2SiF6:Mn4+ phosphor is used in various industrial applications. Similarly, the K3SiF7:Mn4+ phosphor, which has a shorter decay time than K2SiF6:Mn4+, has been newly introduced and has been extensively studied. However, there is still a need to develop chemically stable phosphors than K3SiF7:Mn4+. Here, Rb2KSiF7:Mn4+ is newly proposed as one of the chemically stable materials having a structure similar to K3SiF7:Mn4+. Synthesis of Rb2KSiF7:Mn4+ involves two steps: preparing Rb2SiF6:Mn4+ as a precursor and sintering to produce the final product. A precursor compound, Rb2SiF6:Mn4+, was synthesized by coprecipitation using RbF, K2MnF6 and H2SiF6 in HF solution. And then new Rb2KSiF7:Mn4+ phosphor was successfully prepared using Rb2SiF6:Mn4+ and KHF2 through a solid state reaction under reducing atmosphere. The Rb2KSiF7:Mn4+, Rb substituted 3/1/7 phase, was characterized by X-ray diffraction spectroscopy, scanning electron microscopy, X-ray photoelectron spectroscopy and photoluminescence and compared with the corresponding K3SiF7:Mn4+.

Poster Presentation : **MAT.P-338**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

pH Dependent Energy Transfer in the Fluorescein-Functionalized Au Nanoclusters

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Intracellular pH measurement plays a critical role in bio-applications, especially in diagnosis and drug delivery systems. Here we designed and successfully synthesized a highly sensitive water soluble pH probe, based on a fluorescein-functionalized Au_{22} nanocluster(Au_{22}-AF). Steady-state photoluminescence(PL) measurements have shown that Au_{22}-AF exhibits more than 160-fold pH-contrasting luminescence in a certain pH range. We further defined this phenomenon by transient absorption measurements, which revealed that there are two competing ultrafast relaxation processes in this system: intracore-state relaxation and nonthermalized energy transfer from Au_{22} to fluorescein. Moreover, the latter becomes predominant at a higher pH, which results in that dramatic PL enhancement. Besides, we have monitored similar performance in different sized Au nanocluster systems, which provides wider insight in understanding the multi-functionalized Au nanocluster platforms. Fluorescein-functionalized Au nanoclusters not only exhibit excellent photostability and low toxicity, but also show high pH sensitivity and wide dynamic range, providing a powerful tool for the intracellular process applications.

Poster Presentation : **MAT.P-339**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Enhanced electrochromic properties of Ti doped WO3 films by simple wet-coating method

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WO3 is a representative reducing colored electrochromic material which shows a reversible color change between the blue and the colorless by the redox reaction.It is known that Ti4+ doping into the crystal lattice of WO3 leads to significant surface morphology changes and increases the cycle stability due to stable Ti-O bonding. In this study, WO3 doped with Ti4+(0, 1, 3, 5, 10, 15mol%) was synthesized by simple precipitation method and the electrodes were fabricated by wet coating method to evaluate electrochromic properties.The switching time characteristics of the pure WO3 and Ti doped WO3 films were investigated at the transmittance wavelength of 660 nm by applying a square-wave potential (between –1.0 and 1.0 V). Compared to the pure WO3, the Ti-doped WO3 film showed excellent electrochromism, including large transmittance modulation (71.8%), fast coloring switching speed (10.7s), and excellent cycling durability at a wavelength of 660nm.

Poster Presentation : **MAT.P-340**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and Thermoelectric properties of metal-doped Ternary sulfide

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The thermoelectric (TE) materials have attracted much attention due to needs for potential renewable energy source. The efficient of thermoelectric devices can be evaluated by the figure of merit , $ZT = S^2\sigma T/\kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature and κ is the thermal conductivity. Among the various kinds of thermoelectric materials, sulfide materials are regarded as a promising eco-friendly TE material due to their earth abundant, low-cost and non-toxic elements. In this study, we synthesize metal-doped Ternary sulfide through solid state reaction. We pelletized metal-doped Ternary sulfide with hot press. The crystal structure was investigated with X-ray diffraction and thermoelectric properties by ZEM-3 equipment and NETZSCH LFA 457 MicroFlash™.

Poster Presentation : **MAT.P-341**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Electrochemical Performances of Amorphous Transition Metal Polysulfides for Li-ion Batteries

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Lithium-sulfur batteries are expected to perform high capacity and high energy density. However, there are several drawbacks such as active materials dissolution and shuttle effect of polysulfide. In this work, we synthesize a series of amorphous transition metal polysulfides CrS_3, MoS_5, and WS_5. The resulting polysulfides were tested as cathode materials in lithium-ion batteries. The amorphous phases are expected to be less susceptible to degradation of performance due to crystal structural and volume change during charge/discharge cycles. Among the three polysulfides, molybdenum polysulfide cathode presents the best electrochemical characteristics. The capacity was higher than 500 mAh/g for 50 cycles and the energy density caused by anionic redox processes was 1218 Wh/kg. The deformation and formation of S-S bonds ($S_2^{2-} \leftrightarrow 2S^{2-}$) and the redox reaction of transition metal M^{n+} occurs reversibly in the cycle. These reversible reactions are expected to contribute to suppressing the active material dissolution and shuttle effect, thus increasing the stability and performance.

Poster Presentation : **MAT.P-342**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Highly selective synthesis of organic and inorganic materials *via* solid state reaction using solid methylamine

Sunjoo Kim, Hee Jung Yang, Hee Sun Park, Si Eun Jang, Kyu Hyung Lee, Nam hwi Hur*

Department of Chemistry, Sogang University, Korea

Solid methylamine, methanaminium methylcarbamate, was prepared from the reaction of methylamine with carbon dioxide in an autoclave. The resulting solid was used as a stable, efficient alternative for toxic and gaseous methylamine. Solid-state grinding of solid methylamine and carbonyl compounds produced imines, which were isolated as sole products in over 97% yields. Complete conversions of the solid-state reactions were typically accomplished within a day at room temperature. Reaction rates were enhanced upon increasing the reaction temperature. In contrast, reactions of carbonyl compounds with gaseous methylamine in the presence of solvent afforded imines in moderate yields along with by-products. As a continuing effort to understand the nature of the solid-state reaction with solid methylamine, we have extended this method to synthesize the hybrid organic-inorganic perovskite $(CH_3NH_3)PbI_3$ using solid methylamine. A detailed description of our synthetic efforts will be presented.

Poster Presentation : **MAT.P-343**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

MOF-derived hierarchical porous carbons for supercapacitor applications

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[1]*Applied Chemistry, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*

Metal-organic frameworks (MOFs) can be utilized as a template for fabrication of hierarchically porous carbons that are suitable for electrodes of electric double layer capacitors (EDLCs). In this study, we present a facile method for successful synthesis of hierarchically well-interconnected porous carbons transformed from polymer@MOF composites, which employed for high-performance supercapacitors.

Poster Presentation : **MAT.P-344**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Major Electronic Transition Shift from Bandgap to Localized Surface Plasmon Resonance in Alloy Nanocrystals

Gyeonguk Ko, Kwang Seob Jeong[1,*], Dongsun Choi[1], Jong-ho Choi[1]

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

The phase transition from semiconductor to metal has been of great interest in nanomaterial fields. It is important to understand the phase transition because the quantum confinement effect is differently reflected in the properties of nanomaterials. The major criterion to determine whether the material is semiconductor or metal is carrier concentration. In order to modify the carrier concentration of CdSe host which is well known as p-type materials, the CdxHg1-xSe and CdxAg2(1-x)Se alloy nanocrystals were prepared by cation exchange method.1 The mercury and silver cations induce the self-doping character to the nanocrystals and the self-doped QDs have a higher concentration of carrier compared to other n-type materials.2,3 Quantum dots whose carrier concentra-tion modified with self-doping show the broad range of electrical transitions that varies from bandgap to intra-band transition in the case of CdxAg2(1-x)Se alloy nanocrystals and further shifts to LSPR in the CdxHg1-xSe alloy nanocrystals.

Poster Presentation : **MAT.P-345**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

A Critical Role of the Interlayer Distance of Nanosheets in Tailoring Their Optical and Electronic Properties

Tae-Ha Gu, Seong-Ju Hwang[1,*]

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Despite many advantages of 2D inorganic nanosheets (NSs) as building blocks for hybrid-type photocatalysts, there has been no systematic research about evolutions of the optical and electronic properties of restacked NSs upon the alteration of their interlayer distance. To investigate the correlation between the optical/electronic properties and interlayer distance of restacked NSs, we synthesized a series of intercalative nanohybrids of layered titanate NS and reduced graphene oxide (rGO) NS with various interlayer distances. The interlayer distance of restacked NSs can be finely controlled by employing various n-alkyalmine molecules as intercalants. The increase of interlayer distance via intercalation of long chain n-alkylamine leads to the significant depression of visible light absorptivity and the subsequent depression of photocatalytic functionality, highlighting the weakening of interfacial electronic coupling between restacked titanate and rGO NSs. The present study clearly demonstrates that the intercalative hybridization with various n-alkyalmine molecules can provide an efficient way of tailoring the interfacial electronic coupling between restacked inorganic NSs and their photocatalytic functionality.

Poster Presentation : **MAT.P-346**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

[Withdrawal] 2D Ternary Superlattice of MoS$_2$/RuO$_2$-Reduced Graphene Oxide Nanosheets with Excellent Electrocatalytic Hydrogen Evolution Reaction Performance

Namhee Kwon, Seong-Ju Hwang*

Center for Hybrid Interfacial Structure (CICS), Department of Materials Science and Engineering, Korea

Poster Presentation : **MAT.P-347**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synergistic Effects of Amorphization and Surface Modification on the Electrocatalyst and Li-O_2 Electrode Functionalities of Manganese Oxide

Xiaoyan Jin, Seong-Ju Hwang*

Center for Hybrid Interfacial Chemical Structure (CICS), Department of Materials Science and Engineering, Korea

An efficient way to improve the electrocatalyst performance of manganese oxide is developed by an exquisite control over structural disorder and surface electrophilicity. With or without the anchoring of iodate cluster, two kinds of amorphous manganese oxide nanocrystals with layered δ-MnO_2-type local structure are synthesized by soft-chemical redox reaction between permanganate and reducing agent (LiI or KBH_4). The amorphous MnO_2 nanocrystal with surface-anchored iodate clusters shows much better performances as electrocatalyst for oxygen evolution reaction (OER) and cathode catalysts for Li-O_2 batteries than do both the iodate-free amorphous nanocrystal and well-crystalline microcrystal. The beneficial effect of iodate anchoring as well as amorphization is attributable to the alteration of surface bonding character, the stabilization of Jahn-Teller active Mn^{3+} species, and the enhanced charge transfer of interfaces, which facilitate the rate determining step of OER process. The present study underscores that both structural disorder and well-defined surface are crucial factors for optimizing the electrocatalyst and cathode functionalities of transition metal oxides.

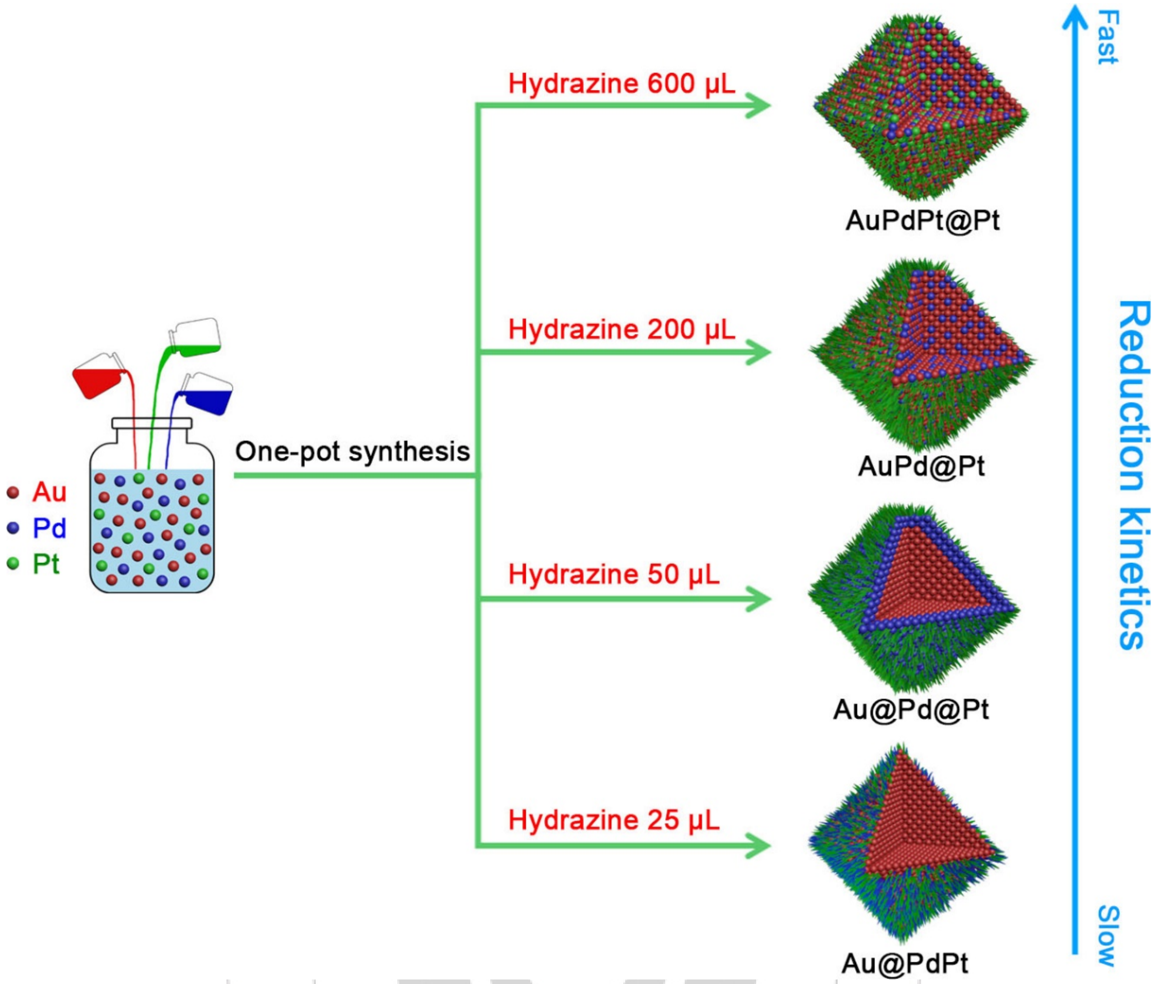
Poster Presentation : **MAT.P-348**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Adjusting the Compositional Structure of Trimetallic Nanocrystals by Regulating Reduction Kinetics for Improved Electrocatalysis

Hochan Ahn, Sang Woo Han*

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

In the present work, we devised an efficient strategy for the systematic control of the spatial distribution of constituent elements in Pt-based trimetallic core-shell NCs, through which NCs with distinctly different compositional structures, such as Au@PdPt, Au@Pd@Pt, AuPd@Pt, and AuPdPt@Pt core-shell NCs, could be selectively generated. The key synthetic lever is the adjustment of the amount of a reducing agent, hydrazine, which can provide fine control over the relative reduction kinetics of multiple metals. Through extensive studies on the influence of the compositional structure of the trimetallic NCs on their electrocatalytic function toward methanol oxidation reaction, we found that the Au@Pd@Pt NCs exhibited considerably enhanced catalytic performance in comparison to the other trimetallic NCs as well as to their binary counterparts, a commercial catalyst, and reported Pt-based nanocatalysts as a result of the optimized surface electronic structure. The present strategy will be useful to design and construct multicomponent catalytic systems for various energy and environmental applications.


Au
Pd
Pt
One-pot synthesis
Hydrazine 600 μL
Hydrazine 200 μL
Hydrazine 50 μL
Hydrazine 25 μL
AuPdPt@Pt
AuPd@Pt
Au@Pd@Pt
Au@PdPt
Fast
Reduction kinetics
Slow

Poster Presentation : **MAT.P-349**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Thermal Insulation Properties of Porous Silica Nanoparticles Synthesized from Water-Glass Precursor

Suguan Jang, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

In this study, we synthesized porous silica nanoparticles with developed pore structure to improve the insulation performance using low-cost water glass. The porous silica nanoparticles has a lot of researches as insulation material because thermal conductivity is drastically decreased due to a large amount of air layer formed inside. However, these materials are manufactured using relatively expensive precursors such as tetraorthosilicate(TEOS), which makes them costly for commercial use. Therefore, we used low-cost water glass as a precursor and used cation exchange resin and surfactant to synthesize materials at relatively low cost. The mesoporous hollow silica with excellent pore structure was compared with general silica to confirm the interaction between the presence of pore structure and the insulation performance according to pore volume. The synthesized materials are analyzed by using N_2-sorption, TEM (transmission electron microscope), SEM./EDX (scanning electron microscope / energy dispersive x-ray) and XRD (X-ray diffraction). After that, the correlation between the volume of the pores and the thermal conductivity was confirmed using Laser Flash Thermal Conductivity Tester.

Poster Presentation : **MAT.P-350**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

The synthesized method 3D-dendritic mesoporous silica using biphase stratification approach strategy for CO_2 adsorption.

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Department of Chemistry, Keimyung University, Korea

In the last few decades, the concentration of CO_2 in the atmosphere had increased rapidly. Many studies have been conducted for CO_2 adsorption and storage. Low-temperature adsorption processes using solid adsorbents such as alkali metal-based materials, metal-organic frameworks, and mesoporous silica. mesoporous silica materials have been studied to take advantages of separation, adsorption, catalysis, and biomedicine due to the high surface and large pore volume. In this study, 3D-dendritic mesoporous silica (DMS) was synthesized using biphase- stratification approach strategy. The dendritic mesoporous silica shows their unique advantage for materials adsorption and loading due to their large pore sizes and radial mesoporous structure. The structural properties of samples were observed by transmission electron microscopy, scanning electron microscope. The organizations of mesoporous silica were analyzed by Xray-diffractometer and the average pore diameter and distribution, and the specific area was calculated by Barret-Joyner-Halender and Brunauer-Emmett-Teller methods, respectively. To improve CO_2 adsorption performance, 3D-dendritic mesoporous silica was impregnated tetraethylenepentamine solution. Adsorption performance of CO_2 according to the concentration of amine solution was analyzed by gas chromatography.

Poster Presentation : **MAT.P-351**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Thin Film of Core-Shell Type MnCoO Spinel Nanocrystals On Porous Carbon Paper Electrode For Oxygen Evolution Reaction

Haeun Lee, Sunglun Kwon, Jong Hyeon Lee*

Department of Chemistry, The Catholic University of Korea, Korea

Development of efficient electrocatalysts for oxygen evolution reaction (OER) is a major topic in commercializing metal-air batteries, water splitting, and solar to fuel production due to the relatively high overpotential and slow reaction rate of the OER reaction. Metal oxides have been intensively studied as non-noble metal oxygen evolution catalysts owing to their attractive durability and activity. Among the various metal oxides, cobalt based-spinel oxides are considered as a promising candidate in OER due to relatively low overpotential, good chemical stability, and earth-abundancy. Additionally, a paper-type carbon electrode can provide large active surface and high conductivity for various OER catalysts. However, synthesis under the high-pH condition and post-annealing at high-temperature for the thin films of crystalline spinel oxide inevitably limit the potential use of carbon paper electrodes in OER. In this study, we suggest a mild aqueous synthesis for the uniform thin film of MnCoO spinel oxide nanocrystals with Mn(II)/Co(II) salts. In the solution synthesis, the size of the nanocrystals increased as the Mn content increased e.g., 13 nm (x=0.0), 23 nm (x=0.005), 50 nm (x=0.05), and 140 nm (x=1.0). The incorporation of Mn into Co_3O_4 dramatically increased the OER performance because the catalytically active Mn cations exclusively substitute the less active Co^{2+} in the MnCoO structure. Also, XPS and ICP inspections suggested an Mn-rich shell/Co-rich core for the MnCoO nanocrystals.

Poster Presentation : **MAT.P-352**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Printing of interdigitated electrodes pattern for open paper-based DMF chip

Sooyong Park, **Veasna Soum, Albertus Ivan Brilian[1], Oh-Sun Kwon*, Kwanwoo Shin***

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Paper is cheaper and more flexible than conventional materials like wafer and can be easily used and discarded. Currently, our lab is studying how to use paper in various fields including lab-on-a-chip technology. In addition, for various experiments using paper, various printing techniques including inkjet printing are utilized.In paper-based DMF chip using Electrowetting on dielectric layer, all droplet manipulations are effective only when fluids are operated between two dielectric layers with channel gaps less than 300 μm to reduce the surface tension. As a result, the liquid volumes are confined to several microliters at most. Moreover, EWOD only works with polar molecules like water and has weak force. To solve these issues, dielectrowetting is applied to achieve creating, transporting, splitting and merging of droplets in open space and with non-polar molecules. If the applied electric field is uniformed, the magnitudes of the electrostatic forces applied on the upper and lower sides of the polarized particles are identical to each other, so the net force applied on the particles becomes zero and the particles do not move. However, when the electric field applied on the particles is not uniformed, the magnitude of the electrostatic forces applied on the particles are different from each other, then the particles are translocated to the dense part of electric field due to the gradient of the electric field. Therefore, in the interdigitated electrodes, due to difference of electric field density, liquid dielectrophoresis occurs. Therefore, the use of liquid dielectrophoresis force can easily control the various motions of droplet underlying chemical reactions on paper based open DMF chips.

Poster Presentation : **MAT.P-353**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

One-Pot Decoration of Gold Nanoparticles On Porous Layered Double Hydroxides By Hydrothermal Treatment

Ho Jung Hwang, Sunglun Kwon[1], Jong Hyeon Lee[1,*]

Department of chemistry, The Catholic University of Korea, Korea

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

In recent years, layered double hydroxides (LDH) have attained significant attention for use in catalyst supports, adsorbents, polymer additives, and cosmetic ingredients due to their large surface area and highly tunable composition. Recently, we have developed a size-tunable decoration method of gold nanoparticles on a nanosheet of LDH materials. The LDH nanosheet was prepared by liquid exfoliation of LDH particles in toxic organic solvents. Also, the synthesis of gold nanoparticles required strong reducing chemicals such as sodium borohydride and hydrazine. In this study, we employed a porous LDH as a support material to decorate the gold nanoparticle in aqueous media. The porous LDH was prepared by washing with aqueous miscible organic solvents and spray-drying. Commercial LDH shows a very low specific surface area of 8.3 m2/g. However, the specific surface area of the porous LDH increased up to 317 m2/g. Additionally, we developed a one-pot synthetic method for the decoration of uniform gold nanoparticles on the surface of porous LDH without reducing chemicals. We found that the hydroxide functionality of LDH plays a crucial role in both reducing the gold precursor and immobilizing the gold metal nanoparticles.

Poster Presentation : **MAT.P-354**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Enhancement of Mechanical Properties of Urushiol@Carbon Nanotube Composite Fibers

Chul jun Yoon, Kyoungsoo Kim[1,*], Youngkwan Kim[2,*]

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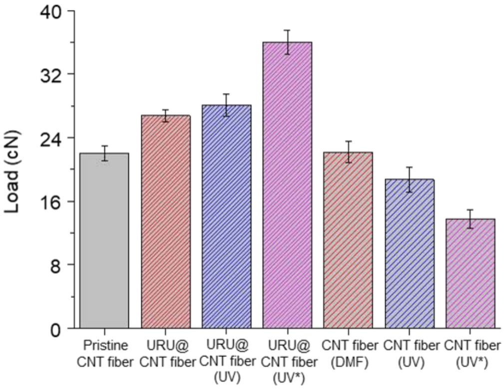
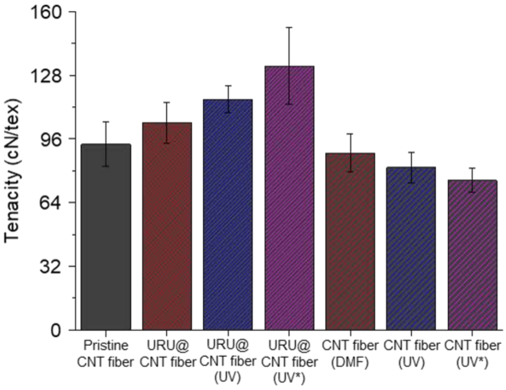
[2] *Korea Institute of Science and Technology, Korea*

Carbon nanotube (CNT) has been extensively studied owing to their excellent electrical and thermal conductivities, and mechanical properties as well as potential for multifunctional materials for various applications. Until now, there have been many efforts for fibrous spinning process of CNTs, leading to the development of various spinning techniques such as direct-, forest- and wet-spinning. Thanks to those efforts, CNT fibers are considered as a next generation material to replace carbon fibers. However, it is still an important issue that the mechanical properties of bulk-scale CNT fibers do not meet those of individual CNT. Here, we report how to enhance the mechanical performance of CNT fibers by using urushiol, a natural UV cross-linkable organic polymer. The surface of the CNT fiber was coated with urushiol and exposed to UV light for a certain time, resulting in the cross-linked CNT fibers with urushiol (Urushiol@CNT fibers). Changes in surface morphology and mechanical properties of CNT fibers by urushiol treatment were characterized by using scanning electron microscopy (SEM) and FAVIMAT to reveal the effect of urushiol coating on mechanical properties of CNT fibers. Based on the experimental results, we found that the urushiol coating on CNT fibers improves their mechanical performance.





* CNT fiber (KIST 2) coated with urushiol (100 mg/mL)
** UV : hand-lamp (254 nm) / UV* : UV curing machine

Poster Presentation : **MAT.P-355**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Highly Emissive Octahedral Rhenium Metal Cluster and Core/Shell Quantum dots with Massive Stokes shift and Its Application on Luminescent Solar Concentrator

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The LSC is a device that employs luminescent dyes to concentrate the sunlight on PVCs (Si cells) attached through the polymer waveguide. It has many advantages such as the possibility of various designs with very high transparency and desirable shape and color. It is also economically competitive and can be processed in the air. We applied octahedral rhenium clusters and quantum dots with free of toxic elements as a luminophore, which has transparency due to the low absorption at visible range and zero-reabsorption due to the massive Stokes shift. The metal clusters, (dMDAEMA)$_4$[Re$_6$S$_8$(NCS)$_6$], prepared by reaction of cesium salt of cluster anions with tetrabutylammonium thiocyanate method were uniformly mixed with PMMA. Also, CuInS$_2$/ZnS core/shell quantum dots, synthesized by a hot-injection method were mixed with polymer which mixed with rhenium cluster. The LSC with highly emissive octahedral rhenium cluster and quantum dots exhibit >80% transparency and high efficiency depending on various concentrations.

Poster Presentation : **MAT.P-356**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

A General Synthetic Route to Atomically Dispersed Catalysts for Revealing Their Catalytic Trends in Oxygen Reduction Reaction

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[1]*Korea Advanced Institute of Science and Technology, Korea*
[2]*Division of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

Atomically dispersed catalysts have recently emerged as a research frontier in catalysis with their maximum atom efficiency and unusual catalytic reactivity. However, a generic strategy toward atomically dispersed catalysts of wide range of compositions is still lacking, which has often limited systematic studies that can unravel the catalytic origins of atomically dispersed catalysts. In the work, we present a generalized synthetic route to atomically dispersed catalysts of precious metals, which consists of “trapping” of precious metal precursors and “stabilizing” them with SiO_2 layers. Through mass spectrometry analyses during activation processes of catalysts, we demonstrated that the “trapping-and-stabilizing” method is capable of impeding the decomposition of a metal precursor, preserving atomically dispersed sites. Five atomically dispersed precious metals (Os, Ru, Rh, Ir, and Pt) catalysts were obtained and served as model catalysts for unravelling reactivity trends of atomically dispersed catalysts for oxygen reduction reaction (ORR). Combining experimental results and density functional theory calculations, we revealed that higher H_2O_2 selectivity was shown in atomically dispersed catalysts compared to their nanoparticle counterparts, which originates from abnormally weakened oxygen binding energies and isolated geometric configurations of atomically dispersed sites. Furthermore, the relative binding energies of *OOH and *O species were identified as determinants that dictate the ORR selectivity of atomically dispersed catalysts. This rational approach for preparing atomically dispersed catalysts can aid in enhancing the understanding their universal catalytic behaviors for ORR.

Poster Presentation : **MAT.P-357**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Cr, W co-doping effect on the phase transition of VO_2

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The Cr^{3+} and W^{6+} doped VO_2 smart films ($V_{0.97-y}Cr_{0.03}W_yO_2$, $0 \leq y \leq 0.1$) have been deposited on sapphire c-plane, (0001). The well known phase transition of the VO_2 film could be modified by the co-doping: The lower valence impurity (Cr^{3+}) makes sharp transition and increases the transition temperature (Tc) by hardening the low temperature lattice of VO_2 (M-type), especially the starting point of metal to insulator shift from 308 K to 320 K by 3% of Cr doping. On the other hand, the higher valence impurity (W^{6+}) makes unclear transition and decreases the (Tc) by the increased hopping site (V^{3+}) of the charge carrier in the lattice -9 K/atomic W %. The sudden changes of optical and electrical properties near ambient temperature were achieved by the co-doping.

Poster Presentation : **MAT.P-358**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Sugar detection of graphitized carbon nanotubes attached with gold particles

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A simple and inexpensive the sugar family (glucose, fructose and sucrose) detection element were prepared by the Au nanoparticles attached to graphitized carbon nanotubes (Au-CNTs), which are fabricated through the carbonization of sucrose based on anodic aluminum oxide (AAO) template. The size of high crystalline AuNPs attached to CNTs have ~26 nm diameter and the graphitized carbon also showed good crystallinities. The field effect transistor (FET) as the sugar family detector was assembled Au-CNTs within a pair of Au electrode on Si/SiO_2 by using the dielectrophoresis. It showed high sensitivity for sucrose but low sensitivity for glucose and fructose, which indicate good sucrose selectivity of FET detector. The larger diameter of CNT(r=250 nm) showed the higher sensitivity than smaller diameter of CNTs (r=40 and 80 nm).

Poster Presentation : **MAT.P-359**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Enhanced lithium storage and rate capability of Mn_3O_4/graphene hybrid with macroporous structure

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Recently, as interest in environmentally friendly renewable energy has increased, a lot of researches have been focused on energy storage systems. Especially, manganese oxide has been actively studied as anode of lithium secondary batteries due to their high capacity. In this study, by utilizing graphene's large specific surface area and excellent electrical conductivity, manganese oxide was hybridized with graphene nanosheets. According to the electron microscopic study, the nanohybrids were formed to maintain spherical hollow structure. Energy dispersive spectroscopic mapping images showed that the manganese oxide nanoparticles were homogeneously distributed in the matrices of graphene layers. Electrochemical charge/discharge tests clearly showed that the nanohybrids had much larger lithium-ion storage capacity than the bare MRGO.

Poster Presentation : **MAT.P-360**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Critical Evaluation of Solid-like Adsorption of H_2 on Porous Materials Using BET Theory: A Molecular Simulation Study

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School of Chemical and Biomolecular Engineering, Pusan National University, Korea

Recently, solid-like adsorption of hydrogen on mesoporous silica material at 20 K has been experimentally observed, but the origin of high-density hydrogen adsorption is still in debate. In this work, GCMC simulations and BET analyses were carried out on four different metal-organic frameworks (MOFs) and a model homogeneous CNT pore (d = 10 nm) to elucidate the origin of solid-like hydrogen adsorption at low temperature. Molecular simulation snapshots were analyzed and compared with the BET area calculated from the adsorption isotherm to test the validity of consistency criteria from BET theory.

Poster Presentation : **MAT.P-361**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Enhanced Adsorption and Photocatalytic Degradation of Organic Dyes by HNTs/TiO_2/La_2O_3 Nanocomposites under UV and Visible Light Irradiation

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

The study of high performance nanocomposites by coating nanoparticles on porous materials has attracted much attention in the field of catalysts and environmental purification. Halloysite nanotubes (HNTs) are naturally occurring aluminosilicates and have a unique structure in hollow form. The inner surfaces of HNTs are Al–OH structures with (+) charge and the outer surfaces are Si–O–Si structures with (–) charge. Due to these properties, HNTs are used to adsorb contaminants. Titanium oxide is applied to various fields such as photocatalyst for decomposing environmental pollutants, electrode for dye sensitized solar cell, and self-cleaning agent. TiO_2 has a wide band gap of 3.2 eV and mainly receives light in the ultraviolet region to decompose organic pollutants. However, due to the small area occupied by UV in sunlight, research to enhance the photocatalytic effect in the visible region is necessary. Lanthanum oxide is reported to increase the photocatalytic effect by increasing the stability of TiO_2 anatase phase and assist electron excitation. We found that HNTs/TiO_2/La_2O_3 nanocomposites increased organic dye adsorption and photodegradation. HNTs are catalyst templates that help adsorb the organic pollutants. La_2O_3 doped TiO_2 exhibits photocatalytic activity in the visible region. HNTs/TiO_2/La_2O_3 nanocomposites were characterized by FT-IR, zeta potential, and FE-SEM analysis. It was found that adsorption amount of rhodamine B in HNTs/TiO_2/La_2O_3 was increased by 62% compared to TiO_2. Photodegradation efficiency of rhodamine B by HNTs/TiO_2/La_2O_3 increased by 36% for 20 minutes under UV irradiation and 16% for 2 hours under direct sunlight. It is a research that is applied to environmental purification by decomposing organic pollutants in waste water.

Poster Presentation : **MAT.P-362**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Conductive Hole Transporting Polymers without dopant for Highly Efficient and Stable Perovskite Solar Cells

Seyeong Lim, Junwoo Lee, Hyuntae Choi, Daehwan Lee, Jihyun Min, Taiho Park*

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We report polymeric hole transport material (HTM) without dopant, which exhibits highly stable and efficient perovskite solar cells (～17.3% for over 1400 h at 75% humidity). The HTM, which is consisted of a random copolymer (RCP), characterized using UV-vis spectrophotometer, cyclic voltammetry, space charge limiting current, and grazing-incidence wide angle X-ray scattering (GIWAXS). The RCP-based perovskite solar cells shows the highest efficiency (17.3%) in the absence of dopants [lithium bis(trifluoromethanesulfonyl) imide and tert-butylpyridine]. The observed efficiency is resulted from a deep HOMO energy level and high hole mobility. In addition, the long-term stability of the device dramatically increased by removing deliquescent or hygroscopic dopants and introducing a hydrophobic polymeric HTM. RCP devices maintain their initial efficiency for more than 1400 hours at 75% humidity, whereas devices made with HTMs with additives do not work after 900 hours.

Poster Presentation : **MAT.P-363**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Mechanistic Studies of CO_2 Cycloaddition in Propylene Oxide (PO): A Density Functional Theory Study

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School of Chemical and Biomolecular Engineering, Pusan National University, Korea

Chemical fixation of CO_2 with propylene oxide (PO) to produce propylene carbonate (PC) is an attractive way to convert CO_2 into valuable chemicals. The rate-limiting step of the reaction is the CO_2 ring-opening step with the activation energy of ~30 kcal/mol. High temperature/pressure is necessary for this reaction to move forward because of the high activation barrier of the rate-limiting step of the reaction. Towards this end, development of a catalyst that can lower the activation barrier of the ring-opening reaction for CO_2 cycloaddition reaction can help lower the operating cost of the reactor and is a highly active area of research, In this work, we carried out DFT calculations on Zn-/Co-ZIF-71 to evaluate the effect of different transition metals on ring-opening mechanism for CO_2 cycloaddition reaction.

Poster Presentation : **MAT.P-364**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Annual meadow grass (*Poa annua*) mediate green synthesis of biologically active silver nanobeads and their biocompatibility evaluation

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Biologically inspired green synthesis of nanoparticles has attracted considerable worldwide attention in the field of biomedical science. Various biological synthesized nanoparticles designed in a unique way to reduce their toxic potencies as compared to chemically fabricated nanoparticles. This is the first report of using common agriculture waste, annual meadow grass *Poa annua*, in the green synthesis of silver nanoparticles (AgNPs). Phytochemical analysis and gas chromatography-mass spectroscopy of *Poa annua* extract depicted ample quantities of reductant materials including flavonoids, phenols and alkaloids which are essential in bioreduction of precursor salts. AgNPs (average size: 49 nm) found stable in different solvent (Deionized water, phosphate buffer saline, dimethyl sulfoxide) for over one month at 4 °C. These biogenic AgNPs are further loaded with a drug (*Euphorbia dracunculoides* plant extract) and coated with starch as a novel drug delivery composite (AgNPs-drug@starch) for cancer therapeutics. The biocompatible nature of AgNPs and AgNPs-drug@starch was analysed using antioxidant assay, hemolysis assay and 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay against (HEK293, A549, SCC7) cell lines. In vivo, AgNPs with highest dose (300 mg/kg) exhibited no significant cytotoxic after 7 days of oral administration. It is concluded that *Poa annua* produced biologically active and biocompatible AgNPs are potential drug career in the field of therapeutics.

Poster Presentation : **MAT.P-365**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Highly Efficient and Thermally Stable Perovskite Solar Cells with Zwitterion interlayer and Polymeric Hole Transport Material.

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Herein, highly efficient and thermally stable perovskite solar cells (PSCs) are reported by introducing a layer of zwitterion molecule over SnO_2 electron transport layer (ETL). This molecule contributes to improving the performance of PSCs mainly in four ways: 1) Enhancing charge extraction inducing shift of work function of SnO_2. 2) Improving electron transport by pulling electrons toward ETL from perovskite layer. 3) Preventing back recombination between charge carriers through the intrinsic dipole in zwitterion molecule. 4) Positively charged nitrogen atom could passivate point defects of perovskite crystal improving both efficiency and stability. With this strategy, the highest power conversion efficiency (PCE) of 21.43% is achieved with doped Spiro-OMeTAD. Moreover, when doped Spiro-OMeTAD is replaced with non-doped polymeric hole transport material (HTM), the 20.5% of PCE is obtained with remarkable thermal stability. This strategy provides a facile way to increase both the efficiency and stability of PSCs.

Poster Presentation : **MAT.P-366**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and Characterization of Murdochite-Type Copper Oxyhalides

Si Eun Jang, Kang Hyun Song, Seok Won Yoon, Hee Jung Yang, Hee Sun Park, Nam hwi Hur*

Department of Chemistry, Sogang University, Korea

The synthesis and characterization of Cu_6O_8MCl (M=Y, In, Dy, Er, Pb) with the murdochite structure will be presented. Murdochite is a mineral with the general formula of $Cu_6O_{8-x}PbX_{2x}$ (X=Cl, Br; x_6O_8] cages and [PbO_8] cubes. Halogen ions are located in elongated [$Cu_6O_4X_2$] octahedra. The Cu_6O_8MCl compounds were prepared by annealing $Cu(NO_3)_2$, $CuCl_2$, and corresponding metal oxide at high temperature in oxygen atmosphere. They were fully characterized by X-ray powder diffraction, thermogravimetric analysis, and SQUID magnetometer. Their structures were refined by the Rietveld method using a GSAS program and their magnetization data were obtained using a SQUID-VSM. In addition, we have investigated on the selective extraction of chloride anions from the Cu_6O_8MCl compounds.

Poster Presentation : **MAT.P-367**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Size-dependent Photocatalytic Activities of Gold Nanoparticles

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Photocatalysts with noble metal nanoparticles referred to plasmonic photocatalysts are receiving increasing interest due to their large absorption cross-section in the visible region. Recently, plasmonic gold nanoparticles photocatalysts researches have been reported to prove electron transfer kinetics, changing in activation energies, and have been used to drive important chemical reaction such as CO_2 reduction. However, the size of gold nanoparticles that used in these researches was fixed around 15 nm, which can readily be synthesized by the Turkevich method. We anticipate that as changing in size of gold nanoparticles, the absorption cross-section and photoelectrochemical potential of gold nanoparticles can be tuned, leading to drive different electron transfer kinetics with previous works. In this study, we demonstrated the influence of plasmonic gold nanoparticles catalyzed chemical reaction as a function of their size. We prepared 4 different gold nanoparticles in size, and monochromatic light source was used to excite the plasmon resonance of gold nanoparticles. To investigate photoreactivity as a function of different size of gold nanoparticles, we monitored Fe^{3+} to Fe^{2+} photoconversion using ferricyanide/ferrocyanide redox couple. On the basis of our experimental results, the correlation between the size of gold nanoparticles and photochemical activities can probably be established.

Poster Presentation : **MAT.P-368**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Structural variation of ultrathin Pt-Co nanowires and their oxygen reduction reaction (ORR) performance

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Pt-based nanocatalysts are widely used for the cathodic oxygen reduction reaction (ORR) in the fuel cells owing to their performance and durability in highly corrosive environment. Among various shaped Pt-based nanocatalysts, nanowires (NWs) showed higher ORR performance due to their structural behavior and higher electrochemically active surface area. Here we present a facile way to synthesize ultrathin one dimensional Pt-Co nanowires using wet chemical method. Two types of Pt-Co Nanowire was formed with or without magnetic field. Characterization of the samples at different synthesis conditions was investigated. It was found that in presence of magnetic field, grain boundary free single crystalline Pt-Co NWs/C were formed which exhibit superior ORR mass activity of 2.54 A $\mathrm{mg^{-1}}_{\mathrm{Pt}}$. Synthesis without magnetic field yield Pt-Co NWs containing grain boundaries, which showed ORR mass activity of 0.92 A $\mathrm{mg^{-1}}_{\mathrm{Pt}}$. Differences in the NWs structure induce different electrocatalytic and magnetic performance, which also effect ORR performance.

Poster Presentation : **MAT.P-369**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Visible Light-Driven Gold Photocatalysts: Comparison of Photocatalytic Activities between Gold Nanoparticles and Gold Nanoclusters

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Department of Chemistry, Yeungnam University, Korea

Plasmonic metal nanocrystals, i.e., Au, Ag, Cu, have been received increasing attention to use as visible light photocatalysts referred to plasmonic photocatalysts due to their unique optical property from localized surface plasmon resonance (LSPR). Although the plasmonic photocatalysts researches have widely expanded in the field, those researches have been limited to plasmonic metal/semiconductor heterostructures or particulate plasmonic metal nanostructures (NPs). Metal nanoclusters (NCs) are a class of ultrasmall nanoparticles in size is perceived as promising materials to use as photocatalysts because of their huge active sites. Unlike nanoparticle photocatalysts, however, the researches of nanoclusters based photocatalysts have not been much reported yet. In this study, we demonstrated the photocatalytic activity between Au nanoparticles (AuNPs) and Au nanocluster (AuNCs) as photocatalysts. We employed ferricyanide/ferrocyanide redox couple as an indicator of our model system. Monochromatic visible light was used to excite the plasmon resonance of Au nanocrystals, and we monitored spectral changing of ferricyanide/ferrocyanide redox couple to determine photogenerated electron transfer rate. We also carried out the power-dependent experiments to kinetic study of Au catalyzed photochemical reaction. We anticipate that our experimental results will provide a clue to develop higher efficient visible-light plasmonic photocatalysts.

Poster Presentation : **MAT.P-370**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Photoluminescence and lasing of bulk Tellurium solid and microcrystals at mid-infrared region

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Tellurium as p-type semiconductor has been of great interest in physics, material science, and nanoscience due to its high thermoelectric performance and photoconductivity. The physical properties of Te crystal have been studied theoretically and experimentally. In particular, Te crystal semiconductors with narrow bandgap (0.33 eV) suggest that Te could be applicable in thermoelectric materials and superconductors at room temperature. However, photoluminescence (PL) of Te crystal, an important potential optical property, has never been measured experimentally at room temperature. Here, we present the PL with narrow full width at half-maximum (fwhm) and lasing in the midwavelength infrared (MWIR) region for Te bulk solid crystal and microcrystals. When decreasing temperature or increasing photoexcitation intensity, MWIR random lasing of the bulk Te crystals is observed at 3.62 μm. In addition, the rod-shaped Te microcrystals synthesized by epitaxial growth on the annealing conditions at 773 K exhibit second harmonic generation (SHG) and third harmonic generation (THG) at MWIR and SWIR, respectively. The strong PL emission intensity and lasing of the Te elemental solid and microcrystals will play a meaningful role as a mid-IR light source, allowing new applications in optoelectronics, infrared photonics, and intensely long-depth penetration bioimaging.

Poster Presentation : **MAT.P-371**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Photoreactivity of Plasmonic Photocatalysts with an Anisotropic Gold Nanostructures

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

Localized surface plasmon resonance (LSPR) of the metal nanocrystal, resulting from the light-to-matter interaction, is greatly considering as a key role in visible light photocatalysts. Many of researches have been reported the enhancement of photocatalytic activities by utilization of LSPR phenomenon of gold nanoparticles. For the face-centered cubic (fcc) gold nanoparticle, the crystal facets are primarily dominated with the low surface energies such as {111} and {100}. Such gold nanoparticles are anticipated catalytically less active than other gold nanocrystals with higher surface energies. In this study, we show the crystal facet-dependent photocatalytic activity with anisotropic gold nanocrystals. We prepared anisotropic gold nanostructures through the seed-mediated method with similar size of gold nanoparticles. We carried out the photochemical reaction with synthesized gold nanostructures and compared it with gold nanoparticles. The synthesized gold nanostructures were characterized by XRD, TEM, and the photoreactivity was measured using UV-Vis spectrophotometer.

Poster Presentation : **MAT.P-372**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

In silico prediction of crystal density for high energy materials using machine learning methods

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[1]*Agency for Defense Development, Korea*

The explosive performance of high energy materials(HEMs) is expressed in terms of detonation velocity and pressure. By the K-J equation, the density of HEMs greatly affects the detonation velocity and pressure. The denser HEMs, the higher explosive performance. The density estimation of HEMs can be used to predict explosive performance with K-J equation. In this study, predictive models were developed using the Quantitative Structure-Property Relationship (QSPR) method that predicts the density of HEMs from chemical structure. Crystal density data was collected from The Cambridge Crystallographic Data Centre (CCDC) and molecular descriptors were calculated from their chemical structures using PreADMET program. Model building of MLR (Multiple Linear Regression) and SVM (Support Vector Machine) were performed by combining feature selection and model validation using forward selection and genetic algorithm. Also the optimization of DNN (Deep Neural Network) model was performed. The robustness and predictability of the model was confirmed by external validation/ y-scrambling and the applicability domain of the individual model was also established. The performance of all models was excellent, and their consensus model will be the prediction model of HEMs with extended applicability domain.

Poster Presentation : **MAT.P-373**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Application of ensemble method for prediction of electric properties of polymer composites

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[1]*Korea Research Institute of Chemical Technology, Korea*

The polymer composites consist of polymer materials, filler materials, and additive, and In order to develop new polymer composite with excellent physicochemical properties, the process of optimizing the material and composition is involved, which is time-consuming and expensive. In this study, we have developed predictive models that predict the volume resistivity, which is one of the electric properties of materials, using the composition ratio of polymer composites. The data used to develop the predictive model was the data collected from literature and patents by KRICT's Chemical Solution Center for several years. Several machine learning methods such as MLR, SVM, deep neural network, random forest, and gradient boosted tree were used as model algorithm, and a single model was compared with various ensemble models. The deep neural network method was the most predictable of the single model, with the gradient boosted tree method using feature engineering technique being the best ensemble model. All models were validated by bootstrap validation and y-scrambling method, to ensure the model's robustness and predictablity. The developed model will be alternative to reduce time and cost of developing polymer composites with desired volume resistivity.

Poster Presentation : **MAT.P-374**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Rhombic dodecahedral Pd@Pt core-shell nanocrystals with Pt {110} shell for enhanced activity towards oxygen reduction reaction

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Numerous studies of strained nanocatalysts have been reported as surface lattice strain has a significant effect on catalytic properties of nanomaterials. However, there are only few studies of strain effect on Pt {110} facet. Here, we report Pd@Pt core-shell rhombic dodecahedra with various number of Pt atomic layers (Pd@PtnL RD (n = 6, 7, 9, 16)) and their influence on oxygen reduction reaction (ORR) activity. Surface lattice strain was quantitatively measured according to the number of Pt atomic layers from high resolution scanning transmission electron microscopy images. We found that Pd@Pt16L RD and Pd@Pt9L have no strain on surface lattice and show higher activity towards ORR than Pd@Pt7L RD and Pd@Pt6L RD which have compressive strain on surface lattice. Among them, Pd@Pt9L RD exhibited the highest specific and mass activities, which were four and three times higher than those of commercial Pt/C catalyst, respectively. We hope that the present work can be extended to other synthetic and catalytic applications.

Poster Presentation : **MAT.P-375**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and Characteristics of Multi-Shell Mesoporous Hollow Silica Nanomaterials with Controlled Shell Thickness

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Department of Chemistry, Keimyung University, Korea

Mesoporous Hollow Silica materials with empty interior and well-defined architectures have a high specific surface areas, low density, high loading capacity and can be potentially applied in drug delivery, nano catalyst, gas adsorbents. Studies of mesoporous hollow silica with multiple shells have actively researched to improve physicochemical performance. In this study, we synthesized multi-shell mesoporous hollow silica nanomaterials (MMHS) and prepared amine-impregnated MMHS (A-MMHS) as an adsorbents for CO_2 adsorption. MMHS were prepared by sol-gel method using polystyrene as a core material and PEG-PPG-PEG(P123) and cetyltrimethylammonium chloride(CTACl) as dual templates and tetraethylorthosilicate(TEOS) as a precursor. A-MMHS were prepared by impregnation method using tetraethylenepentamine(TEPA) as an amine source. MMHS and A-MMHS characterized by using Transmission Electron Microscopy (TEM), FourierTransform-Infrared spectroscopy (FT-IR), N_2-sorption, X-ray Diffraction (XRD) and Gas Chromatography (GC) analysis.

Poster Presentation : **MAT.P-376**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Bi-Te covered nanorods: Facile Preparation with Heterogeneous Precursors and its Computer Tomography Guided Cancer Phototherapy

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Department of Chemistry, Kwangwoon University, Korea

Unprecedented preparation of Bi-Te covered nanorods (BTCNs) were accomplished via one-step simultaneous covering process involving solid and ionic heterogeneous precursors, through hydrothermal environment. The concerted formation of rolled nanorods were achieved by the role of additive, dextrose for proton-coupled reduction pathway. Comparing to conventional tellurium nanorods (TeNRs) without shells, BTCNs showed higher colloidal stability against physiological buffered solutions and lower cytotoxicity against HeLa cells. Moreover, BTCNs exhibited highly efficient photothermal conversion and photocatalytic activity comparable to plasmonic metal nanomaterials under the irradiation of 473, 660, and 808 nm multi-wavelength laser. Finally, prepared BTCNs exhibited multi-potent cancer theranostics in vitro and in vivo in combination with computed tomography (CT) imaging.

Poster Presentation : **MAT.P-377**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Scalable Synthesis of Superparamagnetic Fe_3O_4 Nanoclusters for Bioseparation and Bioimaging

Jeonghyo Kim, Van Tan Tran, SangJin Oh, Jaebeom Lee[1,*]

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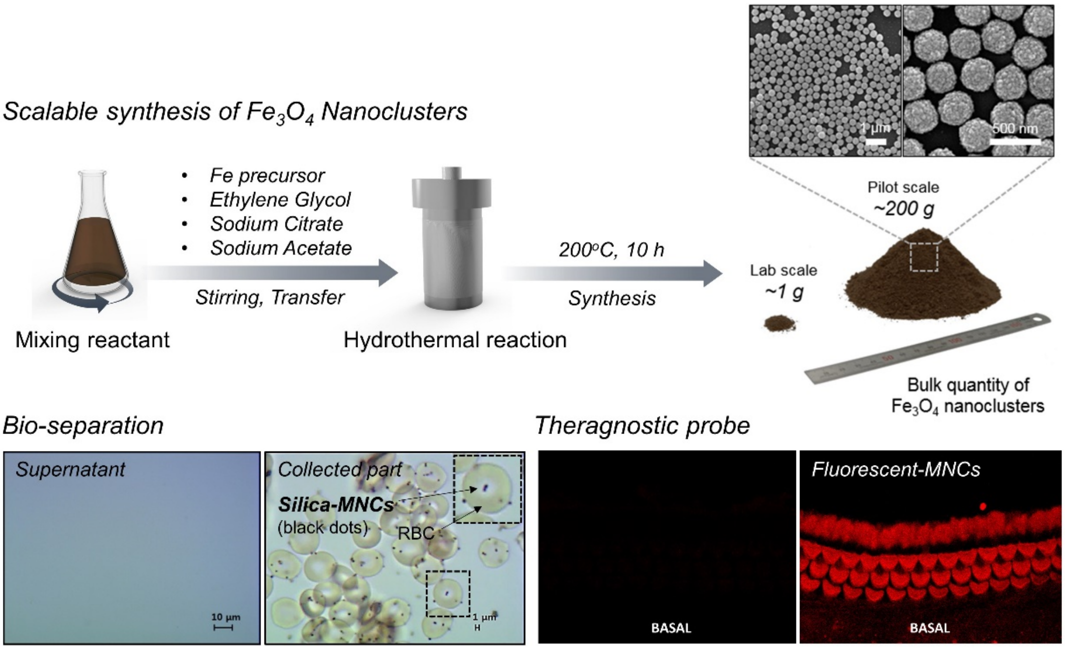
[1]*Chemistry, Chungnam National University, Korea*

Magnetic nanoparticles (MNPs) have had a significant impact on a wide range of advanced applications in the academic and industrial fields. For such applications, the nanoparticles require specific properties, including hydrophilic behavior, uniform and tunable dimensions, and good magnetic properties. However, it remains challenging to achieve a reproducible industrial-scale synthesis of magnetic nanoparticles with such desired properties as precise control of particle growth is difficult. In our current work, we demonstrated a gram-scale synthesis of hydrophilic magnetic nanoclusters based on a one-pot solvothermal system. The synthesized particles have a close-packed superstructure of iron oxide nanocrystals (~13 nm in diameter) that exhibiting hydrophilicity, superparamagnetism, high magnetic responsiveness, and colloidal stability. Additional silica coatings provided further stability and functionality, which was confirmed by in vitro magnetic separation and in vivo fluorescence imaging. These applications verified that the properties of the magnetic nanoclusters fulfilled the various requirements of biological systems. It is expected that this large-scale synthesis of hydrophilic Fe3O4 nanoclusters could be widely used for biomedicine, energy storage, photonics, and catalysis applications, among others.


Scalable synthesis of Fe_3O_4 Nanoclusters
Fe precursor
Ethylene Glycol
Sodium Citrate
Sodium Acetate
Stirring, Transfer
200°C, 10 h
Synthesis
Mixing reactant
Hydrothermal reaction
1 μm
500 nm
Pilot scale
~200 g
Lab scale
~1 g
Bulk quantity of Fe_3O_4 nanoclusters
Bio-separation
Supernatant
10 μm
Collected part
Silica-MNCs
(black dots)
RBC
1 μm
Theragnostic probe
BASAL
Fluorescent-MNCs
BASAL

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **MAT.P-378**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Growth Inhibition of Harmful Cyanobacteria by silver doped molybdenum photocatalyst: Efficiency and Its Mechanisms

Sondavid Nandanwar

Marine Convergence Design Collaboration Course, Pukyong National University, Korea

A novel silver doped molybdenum photocatalyst was prepared by using simple ball milling method and was employed for the inactivation of harmful cyanobacteria for the first time. The effect of photocatalyst on Microcystis aeruginosa under visible light was investigated and a possible mechanism was proposed. The results showed that the synthesized photocatalyst exhibited outstanding performance with a high removal efficiency of chlorophyll a reaching 70% after 4 h and revealed excellent stability under visible light. mechanisms were explored with respect to metal ion release, agglomeration, SEM and algal cell membrane breakage, production of extracellular hydroxyl radical, intracellular reactive oxygen species and lipid peroxidation method. The inhibition of algal growth by photocatalyst was basically attributed to the presence of hydroxyl radical and intracellular reactive oxygen species, with the released Ag+ ion and cell aggregation involved to some extent. Overall, silver doped molybdenum photocatalyst is of great potential in the control of harmful cyanobacterial blooms and the inhibition is specific to the concentration of photocatalyst.

Poster Presentation : **MAT.P-379**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Control of TiO_2 nanostructures from hollow microsphere to microtube

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Tailoring of TiO_2 nanostructures with large surface area, high crystallinity, and controlled shape and pore structures would be a crucial subject in diversifying their applications such as photocatalysts, sensors, photovoltaic and electrochromic devices, and others. Hollow TiO_2 microspheres, which have unique pore structure in the wall and large inner space, have been prepared by a spray pyrolysis technique or by a sol-gel reaction utilizing polymer or silica microspheres as templates. For the first time, in this work, we selectively synthesized hollow TiO_2 microspheres and microtubes in a rich alkylamine environment during solvothermal reaction without the addition of any templates or surfactants. The prepared hollow TiO_2 microspheres and microtubes are composed of highly crystallized anatase TiO_2 nanoparticles without any impurity phase or contamination with inorganic ions. Furthermore, each structure is physically strong and demonstrates extended thermal stability during calcination without pinholes or cracks on its surface. However, controlling the size of hollow TiO_2 microspheres and microtubes still remains very difficult. As mentioned above, hollow TiO_2 microspheres are formed during solvothermal reaction in a rich alkylamine environment, whereas TiO_2 microtubes can be created when both of Ti-alkoxide and alkylamine are further increased. It is worthy of note that the ratio of Ti-alkoxide and alkylamine should be maintained in a suitable range to obtain microtube morphology. If the alkylamine content is too high, TiO_2 microtube structures are broken to nanoparticles.

Poster Presentation : **MAT.P-380**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of Cu-based delafossite nanocrystals for hole-conductor applications

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Several copper based delafossite metal oxides (M = Cr, Al, Ga, Fe, and others) have been known to be a potential p-type transparent conducting oxide material. They are a kind of layered structure, consisting of edge-sharing MO_6 octahedra flattened to the direction of c-axis and Cu(I) cation located in a trigonal coordination environment. Herein, we prepared $CuGaO_2$, $CuCrO_2$, and $CuCr_{1-x}Ga_xO_2$ nanocrystals (NCs) and applied them as hole-transporting material (HTM) of perovskite solar cells (PSCs). Solid solution of $CuGaO_2$ and $CuCrO_2$ in wide range could be readily prepared, because the difference of ionic radius between Cr^{3+} (0.52 Å) and Ga^{3+} (0.62 Å) is very small. Moreover, we except that $CuCr_{1-x}Ga_xO_2$ ($0 < x < 1$) can exhibit better performances than the pure $CuGaO_2$ and $CuCrO_2$ NCs with respect to hole-transporting property and morphology control. In this work, we synthesized $CuCr_{1-x}Ga_xO_2$ NPs by hydrothermal method with soluble metal nitrate salts as precursors. Initially, $Cu(NO_3)_2.3H_2O$, $Cr(NO_3)_3.9H_2O$ and $Ga(NO_3)_3.xH_2O$ were dissolved in pure deionized water. TMAH was used as a mineralizer and ethylene glycol was used as a reducing agent to reduce Cu^{2+} ions. $CuGaO_2$, $CuCrO_2$, and $CuCr_{1-x}Ga_xO_2$ NCs with hexagonal nanodisc morphology were successfully prepared in this work. The prepared $CuCr_{1-x}Ga_xO_2$ NCs provided an improved photovoltaic performance when it was applied as HTM of PSC.

Poster Presentation : **MAT.P-381**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

A Hollow 3D Architecture Formation by Self-assembly of Helical Peptide Mimetic with Poor Macrodipole

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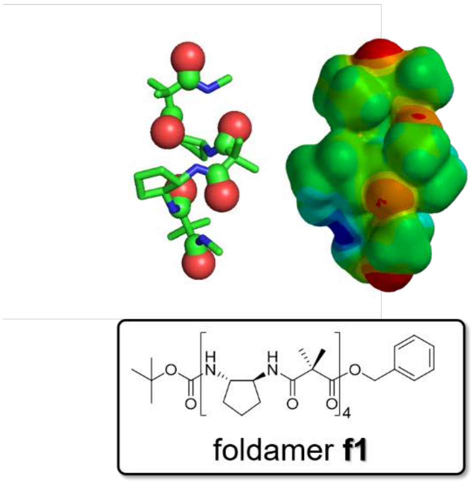
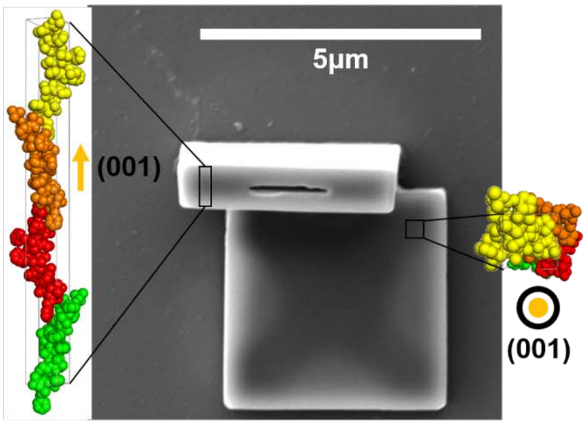
Foldectures, self-assembly of unnatural helical peptide, are well-defined 3D architectures with functional anisotropic surfaces which can serve as potential biochemical materials. Previous studies have shown that physical properties of helical peptides have a strong effect on synthesizing foldectures. However, it was hard to determine whether macrodipole, one of the most important property of helical peptide, is an important factor on foldecture formation. Here, we have synthesized a helical peptide mimetic, foldamer **f1**, which has similiar shape of helical peptide but having less macrodipole. Following a standard foldecture synthesis process, foldamer **f1** self-assembled in a homogeneous foldecture **F1** with a well-defined morphology. Powder X-ray diffraction pattern of foldecture **F1** shows multiple sharp peaks which indicates clear packing structure and was used to solve molecular structure. Based on **F1** structure, it is clear that macrodipole doesn't affect on fast nucleation of foldecture but stable helical molecule having distinct intermolecular hydrogen bond system is the main key.





Poster Presentation : **MAT.P-382**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of Polymeric Drug Carrier Particles with Hierarchically Interconnected Nanopores using PLGA-PEI for Rapid Drug Delivery

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Poly(lactic-co-glycolic acid) (PLGA) is one of the most famous biocompatible and biodegradable polymers, and has been considerably studied in particulate forms in drug delivery systems. In order to improve the functions of PLGA particles, many additives have been used in the synthesis of PLGA particles. Because the rapid drug release using PLGA particles is often essentially required for acute symptoms, the innate slow degradation rate of PLGA causes insufficient timely response to patients. In this study, we synthesized the PLGA particles with hierarchically interconnected nanopores using polyethylenimine (PEI) to enhance the drug release rate by enlarging the surface area of PLGA particles. The synthetic scheme presented in this work is much easier than those reported previously, and results in high size monodispersity. Most importantly, the size and porosity of the nanopores were easily controlled by the amount of PEI during the synthesis. Finally, we used doxorubicin (DOX) and the A549 cell line as a drug and target cells of our drug delivery model system, and evaluated the efficiency of the porous PLGA particles as drug carriers for acute symptoms. During the same incubation time, the DOX-loaded PLGA particles with the hierarchically interconnected nanopores exhibited five times as high efficacy as molecular DOX, which was determined in a series of quantified cell viability experiments.

Poster Presentation : **MAT.P-383**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Charge transfer control by steric effect on the non-conjugated xanthene backbone based donor-acceptor molecule

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We have synthesized a series of non-conjugated xanthene backbone (2,7-di-tert-butyl-9,9-dimethyl-xanthene) based donor(D) and acceptor(A) molecules via a Buchwald-Hartwig, Suzuki-Miyaura cross-coupling reaction. We examined four different diphenylamine donors (F, H Me, OMe) with different electron donating characters to tuning the emission color by charge transfer (CT) control occurring between the donor and acceptor. Based on the solvent dependent emission changes and non-conjugated molecular structure, we have confirmed the emission origin is from the through-space charge transfer (TSCT). The non-conjugated D and A molecules avoid the direct charge transfer and induce of through-space charge transfer, which was identified in the steady state absorption and emission spectra. The Lippert-Mataga plot indicated that these compounds are more affected by steric hindrance than the effect of substituents. From a structural point of view, the donor and acceptor on the xanthene backbone are positioned with co-facial alignment at distances of about 7.5-8.5 Å wherein efficient spatial charge transfer can occur. To understand the structure-properties relationships, DFT and TD-DFT calculations were performed and compare the experimental properties. The results show that the TSCT control based on xanthene molecules have a little effect on color tunable properties.

Poster Presentation : **MAT.P-384**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Distinctive Substituent Effect of 2,7-Bis(*p*-(R)triphenylamino)pyrene on the Intramolecular Charge Transfer

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Intramolecular charge transfer (ICT) process in donor (D) acceptor (A) system with regards to electron push-pull substituents effect and the 2,7-position effect of pyrene were studied. These pyrene-based donor-acceptor-donor (D-A-D) compounds were prepared by palladium catalyzed Suzuki-Miyaura coupling reactions, consisting triphenylamine (TPA) as an electron donor and pyrene (pyr) units as an electron acceptor, respectively. Direct functionalization at the 2- and 7-positions of pyrene triggered the investigation into the electronic structures of 2,7-functionalized pyrene derivatives. By introducing various *p*-(R)-triphenylamine derivatives with electron-donating or electron-withdrawing R groups (R = CN, F, H, Me, and OMe), the energy band gaps of the D–A–D compounds were systematically controlled, and the emission colors were efficiently tuned from blue to green. In the steady state absorption spectra, all compounds exhibit a shape similar to the absorption spectrum of pyrene, which means that all compounds have pyrene properties in the ground state, due to poor π-conjugation by 2,7-position of pyrene. In addition, absorption band around 370 nm a gradual red-shift property was observed in the order of **CN** < **F** < **H** < **Me** < **OMe**, demonstrating that the ICT process is controlled by substituents. In particular, the emission spectra of **CN** compound showed similar emission spectra shape of pyrene, this means that stronger the electron withdrawing group, the more pronounced the pyrene moiety properties. Except the compound **CN**, the other compounds showed the bathochromic shift property with increasing solvent polarity, while compound **CN** can be seen that there is little ICT process. In other words, the emission color appears to be well controlled by the substituents effect, but the **CN** compound has little ICT process, due to the 2,7-position effect of pyrene and the strong electron withdrawing effect.

Poster Presentation : **MAT.P-385**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Bio-inspired surface wrinkle structures templated by self-assembled M13 bacteriophages

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Surface wrinkling can be observed when compressive force is applied to the laminated materials consisting of a stiff film and compliant substrate. The instability caused by the difference in elastic modulus between film and substrate results in the wrinkle surfaces which are minimizing the total energy of the system. In nature, almost every animal has been developed flexion creases on the wrinkling area of the skin to make smooth wrinkling and folding of the skin. For human, palmer creases are very important for delicate motion. Inspired from elaborate and complicated motion of human hand, we introduced bioinspired artificial palmer creases (APC) to achieve well-controlled wrinkle surface. APC was prepared by self-assembly of M13 bacteriophage. M13 bacteriophage is one kind of filamentous bacteriophage. Due to the excellent self-assembly property and genetic engineering technique, M13 bacteriophage have been utilized in many research areas such as colorimetric sensors, bio-imaging systems, energy harvesting devices and optical devices. By controlling self-assembly conditions, we prepared semectically assembled M13 bacteriophage films with different periodicity of defects. When the compressive force is applied to APC, wrinkle surface is formed along with APC. According to the simulation results, strain localization at the defect of semctic film can be observed. Moreover, various types of APC leads to the specific wrinkle surface with different morphologies. We expect that our novel wrinkle surface fabrication method can be used to fabricate unique optical or electrical devices .

Poster Presentation : **MAT.P-386**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Development of a Highly Stable Donor-Acceptor Type Fluorophore Based on Naphthoxazepine Scaffold and Its Applications in Bio-imaging

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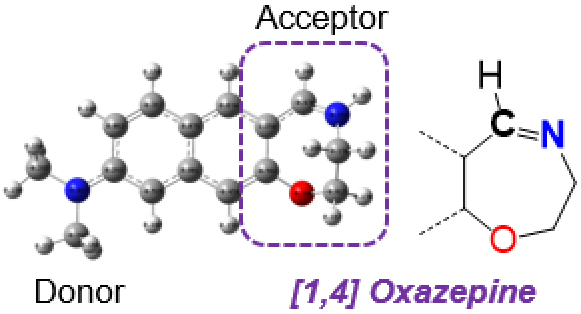
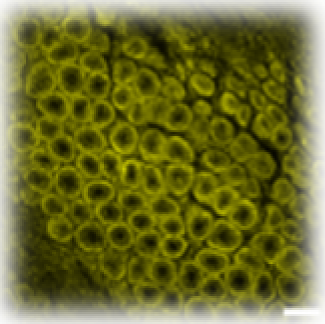
Oxazepines are unsaturated seven-membered heterocyles containing an oxygen and a nitrogen. It has been reported that some oxazepines show interesting biological activities such as antitumor, anti-inflammation, antimicrobiotic acitivites. Especially, medicinally important drugs including Amoxapine, Loxapine, and Nitroxazepine have distinctive structural features consisting of oxazepine backbone with hybridization of two benzene rings. In this work, we developed a new donor–acceptor type napthalene-based oxazepine fluoropore, OXN-1, which exhibits high chemcial stability in harsh conditions. Its exceptional structural stabilities and photophysical properties were thoroughly examined and further explained by quantum chemical calculations. Its bioimaging capabilities for cells with low cytotoxicity were verified. In addition, its deep tissue imaging capability with two-photon microscopy (TPM) was evaluated. These findings may present OXN-1 as a new promising fluorescent probe in biomedicinal application.

Oxazepine-Naphthalene
D-A type fluorophore

- ✓ ***Ultra-stable***
- ✓ ***Lysozyme targeting***
- ✓ ***Low cytotoxicity***
- ✓ ***Two-photon imaging***





Poster Presentation : **MAT.P-387**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Study on the Tungsten Oxide Immobilized in Nitrogen-doped Mesoporous Graphene (NMG/WO_3) nanohybrid

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Department of Chemistry, Dongguk University, Korea

Tungsten oxide (WO_3) was successfully immobilized in nitrogen-doped mesoporous graphene (NMG/WO_3). Tungstate solution precursor was produced by 25 mM of sodium tungstate under acidic aqueous condition (pH 1.67). Tungstate ion having negative charge can interact with positive charge of N^+ site in acid by electrostatic attraction. After annealing at 300 ℃, WO_3 can be obtained. The characterization of NMG/WO_3 nanohybrid was performed by X-ray diffraction (XRD) pattern and field emission-scanning electron microscope (FE-SEM). It has large surface area (396 $m^2 \cdot g^{-1}$) and mesopore (9.53 nm). Amount of WO_3 in composite was estimated by measuring thermal gravimetric analysis (TGA) for 30.08 wt%. To preliminary test the electrochemical performance of NMG/WO_3 nanohybrid as supercapacitor, cyclic voltammetry (CV), galvanostatic charge-discharge (CD) were evaluated in three-electrode system with 6.0 M KOH aqueous solution. The specific capacitance of a nanohybrid is 70 $F \cdot g^{-1}$ at a current density of 3.0 $A \cdot g^{-1}$ and has excellent cyclic stability showing capacitance retention approximately 96 % over 5,000 cycles.

Poster Presentation : **MAT.P-388**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Enhanced gas sensing properties of nitrogen doped mesoporous graphene at room temperature

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[1]*Chemistry, Dongguk University, Korea*

Nitrogen doped mesoporous graphene (NMG) has been synthesized via a hydrothermal method using soft-template, tri-block co-polymer P123 and ammonia as the nitrogen source. During this process, nitrogen doping is achieved simultaneously with reduction of graphene oxide. The obtained NMG has a unique meso-structure, high surface area (1138 m^2 g^{-1}) and a high nitrogen concentration (7.9 at %). These structural features enable the NMG gas sensor to exhibit a high response and better selectivity for NO_2 due to the more active sites on the NMG surface which leads to high interactions between gas molecules and the graphene matrix, and a limit of detection of 0.07 ppm. However the electron-donating gases (NH_3, H_2), demonstrated repulsion between the lone pair of electrons on the NMG surface and the electrons donated from these gases leading to a weak response. The sensing mechanism towards these gases is attributed to the charge transfer between the gas molecules and the NMG sensing material, which shifts the Fermi-level up or down, resulting in an increase and decrease on the electrical resistance respectively. Therefore, electrophilic gases have a strong interaction with the NMG surface compared to the electrophobic gases. Thus, the excellent sensing performance of NMG is attributed to incorporation of N atoms into graphene matrix hence providing a promising platform for electrophilic gas sensing.

Poster Presentation : **MAT.P-389**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

High electrocatalytic performance of three-dimensional nitrogen-doped mesoporous graphene-modified carbon felt electrodes for vanadium redox flow batteries

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

We demonstrate the synthesis of highly electrocatalytic three-dimensional (3D) nitrogen-doped mesoporous graphene-modified carbon felt (NMG-CF) via a facile hydrothermal process, to act as electrocatalysts for vanadium redox flow battery (VRFB). Morphological and spectroscopic studies indicate that the NMG-CF exhibits a uniform distribution of nitrogen atoms (2.19 at.%) and successful N-doping in the form of pyridinic-N, pyrrolic-N, quaternary-N and oxidic-N configurations. NMG-CF show excellent catalytic activity towards VO2+/VO2+ and V2+/V3+ redox couples compared to mesoporous graphene-CF (MG-CF) and activated CF (A-CF), attributed to 3D N-doped mesoporous structures, enhanced specific surface area and rapid charge transfer. Furthermore, N-doping generates defects acting as active sites and alters the electronic and chemisorption properties of MG, hence NMG-CF is more electrochemically accessible than A-CF and MG-CF. Moreover, charge/discharge curves exhibit a high energy efficiency (EE) of 75.1% at a high current density of 150 mA cm-2 in NMG-CF, compared to MG-CF (71.7%) and A-CF (57.1%). Furthermore, NMG-CF shows excellent stability and rate capability (EE ~ 81% after 100 charge/discharge cycles at 100 mA cm-2), with a limiting current density of 275 mA cm-2, indicating the outstanding performance of the modified electrodes during the vanadium ions redox reaction under acidic conditions. The above results reveal applicability of NMG-CF, as a promising advanced electrode material for VRFB.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **MAT.P-390**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis and characterization of nitrogen-doped mesoporous graphene for the removal of volatile organic compounds

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Nitrogen-doped mesoporous graphene (NMG) with interpenetrating porous network was successfully fabricated by hydrothermal process of graphite oxide (GO) and self-assembled triblock copolymer template (Pluronic P123) in the presence of ammonium hydroxide as a nitrogen source. The structure, morphology, chemical components, and porous nature of the obtained NMGs were characterized by X-ray diffraction, scanning electron microscopy, energy dispersive spectrometry, and N_2 adsorption-desorption measurements, respectively. The fabricated NMGs have high BET specific surface area (~ 1107 m^2 g^{-1}), bottle neck like pores with three-dimensional interconnected network, and average pore size with 4.9 ~ 6.3 nm. To preliminary test the performance as a absorbent for volatile organic compounds (VOCs), absorption test using formaldehyde was evaluated in comparison with undoped mesoporous graphene (MG).

Poster Presentation : **MAT.P-391**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

A highly sensitive and multiplexed target DNA detection strategy using DNA-modified magnetic microparticles

Min Ji Hwang, Dongkwon Lim*

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

Magnetic particles have recently received significant research attention owing to their unique magnetic properties and low toxicity. Here, we suggest the DNA-modified magnetic micro particles based strategy for sensitive and multiplexed target DNA detection. The amine-modified DNA was modified on the tosyl-modified magnetic micro particles (MMP) as a target capture probe sequence then, we designed the half-complementary signal probe with fluorescence molecules. The use of MMP facilitates the assay process after mixing with analyte containing possible target DNA sequence. Then, the fluorescence signal intensity can be measured with fluorometer. In this work, the method can simultaneously identify sequences bacteria such as *Escherichia coli*, *Enterococcus faecalis*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. The method showed femto molar sensitivity to bacterial target DNA without interference, which showed a strong potential to identify multiplexing different target bacteria.

Poster Presentation : **MAT.P-392**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

A highly sensitive and stable Radio-isotope embedded AuNPs for PET imaging agent

Wonseok Yang, Dongkwon Lim*

KU-KIST Graduate School, Korea University, Korea

Novel imaging agents with high sensitivity and stability are needed to accurately detect unstable plaques for successful cardiovascular disease. Herein, radio-isotope embedded gold nanoparticles (RIe-AuNPs) can play an important role in the diagnosis of cancer of inflammatory disease as a positron emission tomography (PET) imaging probe1. The RIe-AuNPs were synthesized in straightforward DNA or peptide-based radiolabeling chemistry and additional Au shell formation strategies, leading to high radio-sensitivity and outstanding in vivo stability2,3. Such RIe-AuNPs could demonstrate stable and accurate targeting ability in abnormal blood vessels with densely localized macrophages by modifying specific ligand effective for atherosclerosis. Given such imaging capability to accurately monitor lesion, RIe-AuNPs with specific ligand hold great potential as a highly sensitive and stable PET imaging agent for cardiovascular disease.

Poster Presentation : **MAT.P-393**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Reversible surface chemistry to assemble microchips on the hole array in solution

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Industrially, it is useful to apply chemical reactions that can assemble, combine, and separate micro-sized chips onto a substrate or panel. We applied chemical reactions to assemble, bonding, and maintain microchips on surface-treated substrates, which could be confirmed that the chip remains in the bonded state.After the microchips were assembled, bonded, and maintained on the surface-treated substrate, the separation reaction was performed by using light and chemicals. Especially, synthesized UV-cleavable compound can be chemically decomposed by UV, which is a simple, efficient, and cost-effective method in solution based. The chips binding will proceed quickly and the assembly of the chips efficiently in a solution based chemical reaction. Unlike conventional processes, microchips are combined and separated in solution based and have the potential to be applied to various industries (e.g. display industry).

Poster Presentation : **MAT.P-394**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Synthesis of 2D Complex Nanoframes with dual rims

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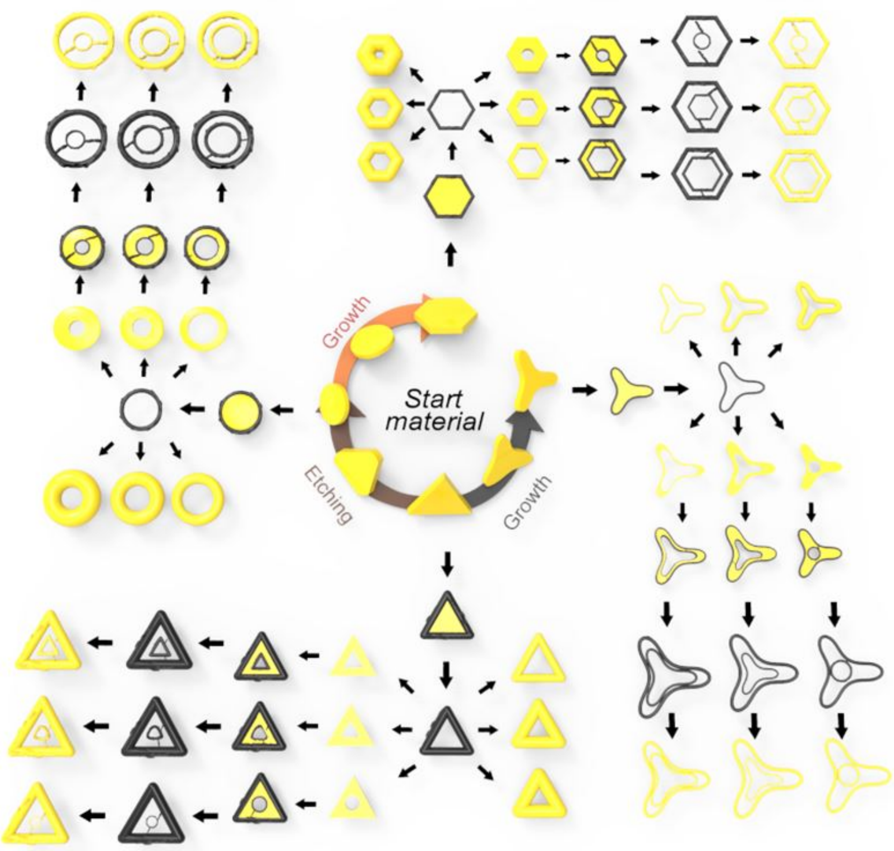
Department of Chemistry, Sungkyunkwan University, Korea

The synthesis of highly complex two-dimensional (2D) metal nanoframes remains a great challenge. Synthetic strategies for preparing 2D metal nanostructure are few, and rational and systematic synthetic pathways to more complicated architectures have not yet been reported. Herein, we demonstrate a multi-stepwise synthetic strategy for complex 2D metal nanoframes with a high degree of intricacy; the strategy leads to a variety of shapes, including rings, triangles, hexagons, and tripods with tailorable single or double frames in a single entity. These nanoframes of high homogeneity could be obtained through multiple steps of selective etching and deposition on certain facets and concentric and/or eccentric regrowth by controlling the mismatches of lattice constants of metals. The resulting nanoframes were highly homogeneous in size and shape and had van der Waals interactions that maximized rim-to-rim contact, allowing them to uniquely self-assemble into large-area superstructures.


Growth
Start material
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Growth

Poster Presentation : **MAT.P-395**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

Fabrication of 2D Tripod Nanoframe Structures for Single-particle Surface-enhanced Raman Scattering Measurement

Jeongwon Kim, Sungho Park*, Sungwoo Lee, Junghwa Lee

Department of Chemistry, Sungkyunkwan University, Korea

Single-particle surface-enhanced Raman scattering has been studied through tailoring intermolecular or intramolecular gap sizes of nanoparticles in order to produce hotspots. Herein, the complexed tripod nanoframe structures for SERS substrate were designed from Au nanoprism solid in wet-chemical method, which can confine the electric fields inside of the nanoframe structure. The tripod shape was formed as the tip regions got grew and edge regions etched out during the shape transformation reaction. AuPt tripod frame structures were successfully obtained through multi-steps that involve Pt rim specific growth reaction and Au etching reaction. In the reaction of Au regrowth, the Au residues existed on the inner side of the AuPt frame induce the eccentric growth. When a little amount of silver ions were added in the reaction, the concentric regrowth is favored because silver ions can reduce the lattice mismatches of Au and Pt. The 2D Au tripod nanoframe structure can serve as a single particle SERS enhancer in the concentric growth with tailorable control of the intramolecular gap.

Poster Presentation : **MAT.P-396**
Material Chemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication of floor polyurethane using environmental –friendly curing agent MBEA

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Department of Chemistry Engineering, Wonkwang University, Korea

MOCA [4,4-Methylene-bis (2-chloroaniline), which has been used as a curing agent for polyurethanes, has been widely used to make polyurethane elastomers with strong mechanical properties. However, MOCA is a solid at room temperature, which is inconvenient to be melted at 110 ℃ or higher when synthesized. Also MOCA structurally attached to chlorine atoms, occuring HCl and phosgene that classified as carcinogens and toxic substances when decomposition at high temperatures. Therefore, it is needed to develop an environmental-friendly polyurethane curing agent to replace MOCA. In this study, we synthesized nontoxic MBEA [4,4-Methylene-bis- (o-ethylaniline)] to substitute chlorine with ethyl group and liquefied at room temperature. Polyurethane elastomers were prepared using MBEA and showed similar properties in hardness and curing time as in the case of conventional MOCA.

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October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **MAT.P-397**

Material Chemistry

Exhibition Hall 1, THU 11:00~12:30

CdHgSe/HgS/CdZnS Colloidal Quantum Dots Exhibiting Bright Short-Wave Infrared Luminescence

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Bright short-wave infrared (SWIR; wavelength = 1000–1700 nm) light emitters provide unique opportunities in various applications including deep tissue biological imaging, telecommunication, and night-time surveillance. Previous researches have introduced SWIR emitters including carbon nanotubes, molecular dyes, rare earth-doped nanoparticles, and semiconductor quantum dots (QDs). However, SWIR emitters with high quantum yield (QY) in the entire SWIR region has not been realized. In this work, we present the fabrication of a new bright SWIR light emitter by synthesizing CdHgSe/HgS/CdZnS colloidal QDs. CdHgSe cores with NIR absorption (700−960 nm) were prepared via Cd-to-Hg cation exchange on zinc-blende CdSe QDs. Then HgS shell with controlled thickness (0.8−1.6 monolayers, MLs) was grown over the CdHgSe core to tune the emission wavelength in SWIR region. Finally, CdZnS layer (typically CdZnS ~4ML) was overcoated to boost QY, increase photostability, and improve their resistance to surface modification necessary for water solubilization. Photoluminescence (PL) spectra showed that our SWIR QDs show narrow-band emission (FWHM

Poster Presentation : **ELEC.P-398**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Attempt to Electrochemical Reduction of Carbon dioxide at LaOCl nanofiber

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In recent years, as the levels of carbon dioxide in the earth’s atmosphere increase the research for electrochemical reduction of CO2 has been studied extensively. Especially, it is well known that some metals have the catalyst efficiency for electrochemical CO2 reduction. For instance the typical CO formation metals reported previously are Cu, Au, Ag, Zn, Pd, Ga, Ni, and Pt. In this study, we synthesized the lanthanum oxide chloride (LaOCl) nanofiber using electrospinning. The existing research direction of LaOCl is roughly divided into two groups, one is display using their luminescent properties and the other is CO or CO2 sensor in gas phase. In contrast to the previous research direction of LaOCl, electrocatalytic properties toward CO2 reduction have been investigated at glassy carbon electrode modified by LaOCl with voltammetry. Morphology and different crystallinity of LaOCl nanofiber by adjusting the calcination temperature were analyzed by field emission scanning electron microscopy (FT-SEM) and X-ray diffraction (XRD). The mean diameters of LaOCl nanofiber in each sample varied from 100-130 nm. The results of the electrochemical study show that our catalyst is effective in CO2 reduction in some degree when calcination temperature should be over 500℃ and sample has some crystallinity.

Poster Presentation : **ELEC.P-399**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Electrochemical Sensor for Drug Detection Using Ion Transfer Reaction at Liquid/Gel Interfaces

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In this poster, we focus on the development of electrochemical sensor chips that measure the concentration of drug ions by measuring the current change with respect to the transfer reaction of the positively charged drug ions (e.g., antibiotics) at a polarized water/polyvinyl chloride-nitrophenyl ether gel interface by applying an electric field. Cyclic and differential stripping plus voltammetry were used to obtain linear relationship between the current versus the drug ion concentration. The real smaple applicability and reproducibility of the developed sensor are currently being investigated.

Poster Presentation : **ELEC.P-400**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Influence of super activation on Nanoporous Au in alkaline solution

Gahyun Kim, Jongwon Kim*

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In alkaline solution, the oxidation peak can found between 0.7 V and 1.1V (vs. Hg / HgO) before the oxygen evolution reaction (OER) at Au surface. This peak is the result of super activation. Super activated surfaces relate to the monomeric Au hydroxyls, which appear to be transient and be regarded as intermediates of β-oxides. Subsequently, Au hydroxyls form the peroxy. During the peroxy decomposition, oxygen is produced in the surface oxide layer. That is, OER occurs earlier than expected potential. Consequently, super activated Au can be used in the study of developing OER catalysts. In this work, Super activation results were observed using an electrode with a porous surface of Au. To create porous surface, Nanoporous gold (NPG) was produced using anodizing method that applied positive potential to Au. As a result of this study, It was confirmed unique transient response in the gold electrode, which is a porous surface. We also identified changes in peak current of transient response due to surface area changes in NPG. And then various methods of super activation for increasing the peak current were applied to NPG and we observed peak change phenomenon. And found the most effective super activation method for NPG electrodes.

Poster Presentation : **ELEC.P-401**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Fabrication of an Amperometric Microsensor for Simultaneous Measurement of Nitric Oxide, Carbon Monoxide and Hydrogen Sulfide

Sunghwa Seo, Youngmi Lee*

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Nitric oxide (NO), carbon monoxide (CO) and hydrogen sulfide (H_2S) are well known as endogenous neurotransmitters in mammalian cells. However, there are still controversy in the way that they are related one to another when they transmit the neuronal signals in brain. Therefore, a triple sensor is developed to establish their functional relations through the simultaneous measurements of these three gases in biological environments.In this presentation, we demonstrate the fabrication of an amperometric microsensor for the concurrent measurement of NO, CO and H_2S. This sensor has three platinum (Pt) working electrodes: 50, 76 and 50-μm diameter Pt microdisks (denoted as WE 1, 2 and 3, respectively) in a three-barrel glass capillary. WE 1 has a bare Pt disk and covered with NO selective membrane. Both WE 2 and 3 are electrodeposited with different metal nanoparticles after Pt disks are etched electrochemically. Then, the surface of WE 2 is loaded with CO selective membrane. And, WE 3 is coated with an electropolymerized film. Finally, this sensor is characterized in terms of the sensitivity by measuring the currents at WE 1, 2 and 3 responsive to NO, CO and H_2S concentration increases at each optimized applied potential. The selectivity of the sensor for the individual targeted gases over common biological interfering species are also confirmed. The feasibility of the prepared NO/CO/H_2S triple sensor to distinguish three gases in biological environments is also studied aiming at determining the relationship of them in biological systems. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2017R1A2A2A14001137).

Poster Presentation : **ELEC.P-402**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Electrospun Gold-Ruthenium Alloy Nanofibers: An Efficient Bifunctional Catalyst for Overall Water Splitting

Taehui Kwon, Areum Yu, Chongmok Lee, Youngmi Lee*

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

Hydrogen (H_2) is one of the purest and renewable energy sources having the outstanding advantages of high energy storage density and sustainable reaction products. Electrochemical water splitting including two reaction systems, the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER), has been regarded as one of the important ways to gain H_2 gas from aqueous solutions. Hence, searching for a bifunctional catalyst being useful for both OER and HER with high activity, efficiency and stability is critical.In this presentation, AuRu alloy nanofibers have been successfully synthesized via electrospinning, calcination and the subsequent reduction process. We confirmed the reduction of Au/RuO_2 nanocomposites to AuRu alloy nanofibers and compared the physical properties of AuRu alloy nanofibers with those of pure Au and Ru characterized by XRD and XPS. Also, the morphologies of the Au/RuO_2 nanocomposites and AuRu alloy nanofibers were verified by FE-SEM and TEM. In electrochemical analysis, OER and HER activities of the synthesized AuRu nanomaterials were measured by rotating disk electrode (RDE) voltammetry in 0.5 M H_2SO_4 aqueous solution. The Tafel plots which represent the reaction kinetics for OER and HER were gained by the corresponding RDE curves. In overall comparison, AuRu alloy nanofibers indicate better catalytic performances toward OER and HER than those of Au/RuO_2, RuO_2, Ru, commercial Pt and Ir. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2017R1A2A2A14001137).

Poster Presentation : **ELEC.P-403**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Electrofibrous Nickel-Rhodium Oxide Nanocomposites for Efficient Electrocatalytic Oxygen Evolution Reaction.

Dasol Jin, Areum Yu, Youngmi Lee*, Myung Hwa Kim*, Chongmok Lee*

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

In the fuel cell systems, the numerous OER catalysts have been synthesized, but noble metal-based electrocatalysts (NMEs) have become the most practical electrocatalysts in terms of durability despite their high cost. It is thus necessary to synthesize catalysts by mixing the cheaper metals with noble metals. The activity of the catalysts is also influenced by the crystallinity whether crystalline or amorphous. It is often reported that amorphous form has more unsaturated sites than crystalline structure. In this study, we have synthesized mixed Ni-Rh oxide nanocomposites, $Ni_xRh_{1-x}O_y$ ($0 < x < 1$), for cost-effective OER NMEs through electrospinning and calcination process by controlling the metal molar ratio. The morphology and catalytic activity have been varied depending on mixing ratio and crystallinity. The morphology and composition of $Ni_xRh_{1-x}O_y$ have been characterized by a field emission scanning electron microscope (FESEM) equipped with an energy dispersive X-ray spectrometer (EDS), high-resolution transmission electron microscopy (HRTEM) and X-ray photoelectron spectroscopy (XPS). Electrochemical measurements for OER have been performed using electrochemical analyzer with RDE in N_2-saturated 1 M NaOH aqueous solution. The support by the National Research Foundation of Korea (NRF), NRF-2019R1F1A1059969 for CL and NRF-2018R1A6A1A03025340 for YL and KMH, is gratefully acknowledged.

Poster Presentation : **ELEC.P-404**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Dry-deposition of LiNbO3 or Li2ZrO3 on LiNi0.6Co0.2Mn0.2O2 assisted by resonant-acoustic technique for all-solid-state lithium batteries

Youngjin Kim, Kwang Sun Ryu*

Department of Chemistry, University of Ulsan, Korea

The LiNbO3 or Li2ZrO3 nanoparticles were coated on LiNi0.6Co0.2Mn0.2O2 (NCM) cathode material (NCM) by resonant-acoustic coating technique for all-solid-state lithium batteries (ASSLB). We have produced LiNbO3 (50~100 nm) or Li2ZrO3 (30~60 nm) nanoparticles, which are the suitable electrode coating agents since it can suppress direct contact sulfide-based solid electrolyte and decrease contact loss along with elimination of the space-charge layer. ASSLB using LiNbO3 or Li2ZrO3-coated NCM materials showed higher capacity than bare NCM. X-ray diffraction patterns showed the same peak separations and lattice parameters as bare NCM. The images of SEM and TEM were analyzed with electron dispersive spectroscopy mapping, which represents homogeneous coating with a uniform LiNbO3 or Li2ZrO3 layer of 50 ~ 200 nm. XPS measurements revealed that the surface of NCM had two different O1s peaks, Nb-O peak, and Ni, Co, Mn, Nb peaks. Electrochemical studies on bare NCM and LiNbO3 or Li2ZrO3 coated NCM materials were elucidated using electrochemical impedance spectroscopy and galvanostatic cycle performances by ASSLB cells with c-rate performances. Especially, the 3 wt.% LiNbO3-coated NCM exhibited capacity retention of 84% at a current density of 15 mA/g during 20 cycles, while that of the bare NCM exhibited capacity retention of 16.1%.

Poster Presentation : **ELEC.P-405**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Highly disperse Palladium nanoparticles: synthesis and the role of pyrrolic and pyridinic nitrogen on reduced graphene oxide boosting superior electrocatalytic activity for ORR

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Chemistry, Chonnam National University, Korea

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The present study shows 3-aminomethylpyridine (AMP) functionalization of reduced graphene supported palladium nanoparticles (AMP-rGO-Pd) for the catalytic oxygen reduction reaction (ORR) in alkaline media. The as-prepared AMP-rGO-Pd nanocomposite was characterized using X-ray diffraction, transmission electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy. This study strongly indicated that the covalent functionalized reduced graphene oxide contains the nitrogen group in the pyridinic form where the palladium (Pd) nanoparticles distributed homogenously on the 3-aminomethylpyridine functionalization of reduced graphene (AMP-rGO). Also, X-ray photoelectron spectroscopy demonstrated that the reduction process was performed successively with the increasing C/O ratio from 0.49 to 1.25. The obtained crystalline feature of as-prepared AMP-rGO-Pd from X-ray diffraction (XRD), it was also worth noting that the highly dispersed palladium nanoparticles are well set on the covalent functionalization graphene oxide. The catalytic performance of AMP-rGO-Pd was examined through cyclic voltammetry, linear sweep voltammetry, rotating disk electrode, and rotating ring disk electrode techniques in 0.1 Molar KOH solution. The AMP-rGO-Pd catalyst showed superior ORR onset potential, higher peak current density, remarkable methanol tolerance as well as magnificent stability in case of alkaline media. Moreover, AMP-rGO-Pd exhibited a four-electron reduction pathway for ORR with minor hydrogen peroxide (H2O2) yield due to the synergistic effect shown by AMP-rGO and highly dispersed Pd nanoparticles.

Poster Presentation : **ELEC.P-406**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Galvanic Displacement Reaction as a Versatile Approach to obtain the Free-standing Gold Nanoflakes on Prussian blue Surface and Its Electrochemical Applications

Juwon Jeong, Manivannan Shanmugam, Kyuwon Kim*

Department of Chemistry, Incheon National University, Korea

Galvanic displacement reaction was used to obtain highly stable and Free-standing gold (Au) nanoflakes (NFs) over the pre-electrodeposited Prussian blue (PB) nanostructures (NSs). Amine functionalized silicate sol–gel matrix was used as a solid support for electrodepositing PB NSs, prior to Au deposition. Physiochemical and electrochemical characterizations were carried out to reveal the morphology and electrochemical stability of the PB-Au NFs. Various controlling parameters to tune the Au NF's size, shape and identify the growth mechanism such as Au precursor concentration and deposition time have been studied. The fabricated PB-Au NFs electrode was used to construct the amperometric sensor for Hydrogen Peroxide (H_2O_2). Furthermore, present electrochemical sensor has exhibited improved performance in the presence of commonly encountered interferences at the physiological conditions.

Poster Presentation : **ELEC.P-407**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Highly Elastic Polyrotaxane Binders for Mechanically Stable Lithium Hosts in Lithium-Metal Batteries

Dong-Joo Yoo, Jang Wook Choi*

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

In an attempt to overcome the longstanding hurdles of lithium metal anodes with unparalleled specific capacities, conductive scaffolds that can take up lithium have been lately investigated with great attention. Carbon nanotubes (CNTs) are ideal units to constitute such scaffolds because their one-dimensional nanostructures can efficiently percolate a conductive network while plating lithium through their internal pores. However, CNT networks are liable to rupture upon lithium deposition due to the generation of substantial stress. Here, we report CNT scaffolds with enhanced mechanical properties by incorporating molecular pulley binder containing a small amount of polyrotaxane (5%) cross-linked to the conventional polyacrylic acid binder. The pulley binder links functionalized CNTs via hydrogen bonds, sustaining the mechanical integrity of the expanding CNT network at a current density of up to 6 mA cm^{-2} and even with an areal capacity of up to 6 Ah g$^{-1}_{\mathrm{cnt}}$. The polyrotaxane in the pulley binder imparts elasticity to the CNT network originating from the ring sliding motion. The improved mechanical stability of the CNT network induces lithium to be uniformly plated/stripped into/from the network pores during repeated cycles. As a result, the molecular pulley binder-incorporated CNT network exhibits considerably improved cyclability in lithium-copper asymmetric cells and full-cells paired with olivine-LiFePO$_4$, compared to the binder-free and non-elastic binder counterpart. This investigation reveals that the integration of elastic binders in conductive lithium-uptake scaffolds can be an important step forward in realizing high performance lithium metal batteries.

Poster Presentation : **ELEC.P-408**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Improving cycle performance of Li-O_2 batteries by immobilized TEMPO on cathode

Ji Hyeon Kang, Inho Nam[1,*]

Chung-Ang University, Korea
[1]*Chemical Engineering & Materials Science, Chung-Ang University, Korea*

The rechargeable lithium-oxygen (Li-O_2) batteries have received significant attention as a next-generation energy storage system with high capacity because of its high theoretical energy density, which approaches 3500 Wh kg^{-1}. However, addressing low energy efficiency and poor cycle performance problems during their practical applications of Li-O_2 batteries still remains challenging. Here, we present a novel Li-O_2 battery system by immobilizing 2,2,6,6-tetramethylpiperidinyl-1-oxyl (TEMPO) on the cathode, which can participate in the redox mediator without undergoing self-discharge, thereby improving the energy efficiency and cycle stability. The TEMPO-immobilized air cathode is prepared by simple dip coating method, in which polydopamine is used as a linker. In this method, the immobilized TEMPO on the cathode inhibited the degradation of TEMPO at the Li metal anode and could extensive Li_2O_2 oxidation over repeated cycles. Therefore, the use of an immobilized TEMPO as our rational strategy will provide a new perspective and breakthrough for the practical applications of Li-O_2 batteries.

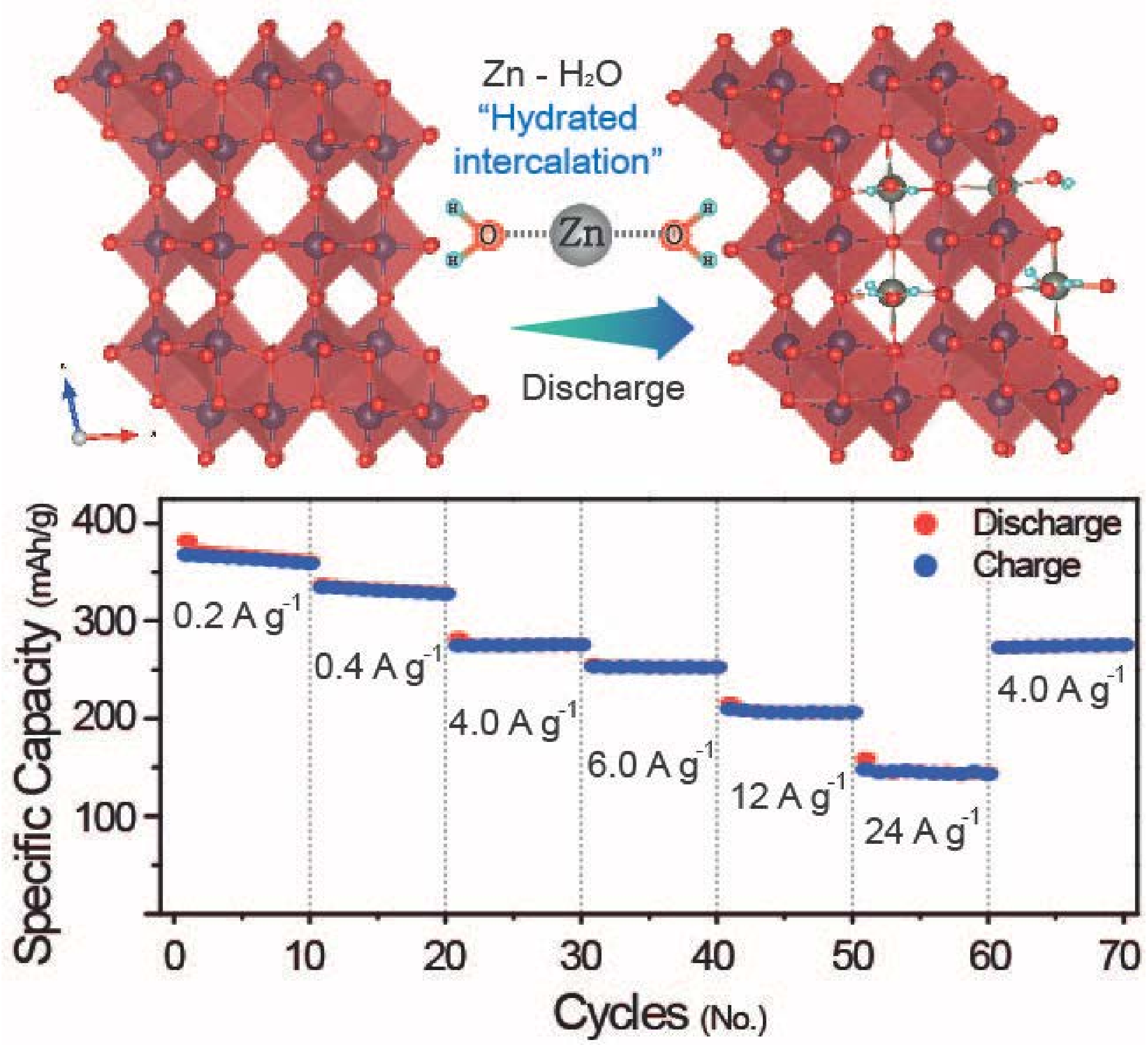
Poster Presentation : **ELEC.P-409**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

High Performance Aqueous Zinc Ion Batteries Mediated via Hydrated Intercalation

Jaeho Shin, Jang Wook Choi*

Chemical and Biological Engineering, Seoul National University, Korea

Aqueous zinc ion batteries (AZIBs), composed of a zinc (Zn) metal anode paired with a metal oxide cathode, are promising candidates for post lithium ion batteries. The bivalence of Zn opens up possibilities for multi-electron redox, which has spurred a fierce search for suitable cathode materials (namely metal oxides) that intercalate Zn^{2+} ions. Despite the recent rise in publications, however, little is known about the intercalation dynamics of Zn^{2+} ions. As such, there is much room to explore the interaction between these ions and their host cathode. In this respect, we focus on a type of vanadium oxide, V_6O_{13}, not only as an electrochemically promising material, but also as a platform with which key Zn^{2+} intercalation parameters can be elucidated. Electrochemical results are correlated with a series of synchrotron XAFS/XRD studies along with DFT calculations to understand the underlying reaction mechanisms. Interestingly, we find that 'hydrated intercalation' is crucial to facilitating Zn^{2+} intercalation kinetics. In this presentation, I will correlate the electrochemical properties with the structural changes of the cathode and explain how water comes into play during this process.


Zn - H₂O
"Hydrated intercalation"
H
O
Zn
O
H
Discharge
Specific Capacity (mAh/g)
400
300
200
100
Discharge
Charge
0.2 A g⁻¹
0.4 A g⁻¹
4.0 A g⁻¹
6.0 A g⁻¹
12 A g⁻¹
24 A g⁻¹
4.0 A g⁻¹
0
10
20
30
40
50
60
70
Cycles (No.)

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ELEC.P-410**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

In-Situ Synthesis of Bi_2S_3 Nanowire on Bi_2MoO_6 for Highly Improved Photoelectrochemical Performance

Jihyeon Kim, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Single-crystalline Bi_2S_3 nanowire array (Bi_2S_3NWA) was synthesized via an in-situ hydrothermal reaction on the surface of the Bi_2MoO_6 film. Because there was no extra addition of the Bi^{3+} source during the process, the Bi_2MoO_6 layer acted as a substrate as well as a Bi^{3+} source for the growth of Bi_2S_3 nanowires. Compared to the other Bi_2S_3 electrodes, the resulting Bi_2MoO_6/ Bi_2S_3NWA composite showed enhanced photoelectrochemical (PEC) activity. The origin of this enhanced activity is mainly attributed to the enhancement of charge separation on the Bi_2S_3 NWA layer, due to the effective photogenerated electron transfer from the Bi_2S_3 conduction band to that of Bi_2MoO_6. Furthermore, the single-crystalline Bi_2S_3 nanowires can provide a fast electrical pathway to Bi_2MoO_6 through a single domain of nanowires.

Poster Presentation : **ELEC.P-411**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Modification of Oxygen Reduction Electrode with Gold Nanocluster

Hanseok Yi, Kyuju Kwak, Young Lim Byeon, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Oxygen Reduction Reaction (ORR) is a key reaction of fuel cell that is the most important energy storage device in green chemistry. Many researchers have made effort to positively shift the onset potential (Eonset) of the ORR and to satisfy 4 electron pathway (direct pathway) in the reaction. Recently, metal nanoparticles have attracted much attention due to their different optical, electrochemical and ORR catalytic properties from bulk metals. Unlike relatively large gold nanoparticles, ligand-protected gold nanoclusters that have a size of less than 2 nm show a redox activity like molecules. In this presentation, we prepared a well-modified electrode using Au25(C6S)18 (C6S=hexanethiol), Nafion and multi wall carbon nanotube (MWNT). In the modified electrode (Au25/Nafion/MWNT), Au25 and MWNT act as redox mediator and electronic conductor, respectively. The Eonset of the ORR in Nafion/MWNT electrode had -0.4 V vs. Ag/AgCl. However, Au25/Nafion/MWNT electrode positively shifted 200 mV than w/o Au25 electrode due to the redox mediator effect of Au25. In addition, we observed that the number of electron is 3.77 (n=3.77) in the ORR with Au25/Nafion/MWNT electrode, unlike Nafion/MWNT electrode had 2.08 (n=2.08) using by RDE.

Poster Presentation : **ELEC.P-412**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Functional Blocking Layer of Twisted Tungsten Oxide Nanorod Grown by Electrochemical Anodization for Photoelectrochemical Water Splitting

Pran Krisna Das

Advanced Chemicals & Engineering, Chonnam National University, Bangladesh

The twisted WO3 nanorod (T-WO3 NR) photoanodes are potential candidates for the anodic part of a solar water-splitting device that produces hydrogen fuel and oxygen from water. The twisted WO3 nanorods (T-WO3 NRs) were grown via the electrochemical anodization of tungsten foil in a fluorinated-based electrolyte and the morphology of the films was controlled by the anodization conditions. The synthesized WO3 layer was composed of two distinct layer; the twisted WO3 nanorods (T-WO3 NRs) as an active layer for the PEC reaction and another compact WO3 (C-WO3) layer which acts as a blocking layer (BL) for the charge transport. As increasing the anodization time, the thickness of the twisted WO3 nanorods (T-WO3 NRs) layer approach to be almost same to approximately 700 nm, but the blocking layer is gradually increased 91 nm at 1 min to 633 nm at 120 min in post-thermal annealing. Unexpectedly, the anodic WO3 film having the compact layer with a thickness of about 475 nm exhibited the highest PEC performance, corresponding to the photocurrent density (J) of 0.75 mA/cm2 at 1.23 V vs. reversible hydrogen electrode (RHE) (abbreviated as 1.23 VRHE), subsequently followed by the anodic WO3 film having a less thick compact layer. This means that the C-WO3 layer promotes the charge transport and suppresses the charge recombination underneath the T-WO3 NR layer, demonstrated by the UPS and XPS analyses in depth profile. Furthermore, the etched T-WO3 NR film using 0.03 M NH4OH solution showed a little bit improved J value, resulted from the increased active area for the water oxidation reaction. Eventually, the functionality of compact layer as well as the surface modification by the wet etching process would be discussed in detail.

Poster Presentation : **ELEC.P-413**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Efficient oxygen evolution reaction of hollow cobalt mesospheres improved by corrosion reactions

Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Although a number of anodic materials have exhibited catalytic activity approaching that of iridium (or ruthenium) oxide catalysts for the electrochemical water splitting, research demand for new catalyst development is constantly required. The electrochemical water splitting has long been considered a promising approach to producing clean hydrogen fuel using renewable energy sources. The hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are the major half reactions occurring in the cathode and the anode respectively in the electrochemical water splitting reaction. Herein, we develop a cost-effective and new corrosion method for transforming hollow cobalt mesospheres into highly active and stable catalysts for OER. The Co catalysts obtained by corrosion reaction were characterized by X-ray diffraction, transmission electron microscopy, and scanning electron microscopy. We also investigate the electrocatalytic activity of the Co catalysts for OER and compare them with commercial carbon-supported iridium. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614

Poster Presentation : **ELEC.P-414**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

2nd Generation Fourier Transform Electrochemical Impedance Spectroscopy (FT-EIS) with Commercial Potentiostat

Long Ha Duong, Kyungsoon Park, Seongpil Hwang*

Department of Advanced Materials Chemistry, Korea University, Korea

The development of 2nd generation Fourier Transform Electrochemical impedance spectroscopy (2G FT-EIS) has enabled fast measurement time and time-resolved EIS. The requirement for a special home-built electrochemical system, however, has been a major challenge for 2G FT-EIS to be applicable widely. Herein, we report a facile modification approach to commercial potentiostat, which has adequate power due to modern electronics and software development, to allow 2G FT-EIS without expensive frequency response analyzer (FRA) module and sophisticated home-built equipment. The comparison of EIS data from our new method and conventional methods will be presented.

Poster Presentation : **ELEC.P-415**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis and application of polycationic ruthenium redox polymer mediator for detection of glucose using glucose dehydrogenase(GDH).

Chang Jun Lee, Ryang Hyeon Kim[1], Subin Park[1], Young Bong Choi, Hyug-Han Kim[*]

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

Glucose amperometric sensor used mediators for electron-transfer between electrodes and enzymes. Complexes of the group VIII metals iron (II), ruthenium (II) and osmium (II) have been synthesized and characterized electrochemically with respect to their ability to act as electron-transfer mediators for redox enzymes. We used FAD glucose dehydrogenase (FAD-GDH) as redox enzyme to selectively measure glucose. FAD-GDH was less activity than GOx and did not react well with cationic mediators. But we have developed Polyvinylimidazole complex of [Ru(dam-bpy)2Cl]+/2+ that is cation and reacts well through different glucose concentration at 0-20mM in 1X PBS. We checked characterization of chemical structure with 1H-NMR, FT-IR, UV-VIS, CV and electrochemical properties with CV, multi-potential step. Finally, we studied cationic ruthenium mediator for application of glucose sensor using FAD-GDH.

Poster Presentation : **ELEC.P-416**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Fe_2O_3 Nanoparticles Coated by N-doped Graphitic Carbon Using Dopamine as an Anode Material for Sodium-Ion Batteries

Jungwook Song, **Jongsik Kim***

Department of Chemistry, Dong-A University, Korea

The increasing studies about the renewable energy technologies have been urged the development of the new power supplying systems to surpass lithium-ion batteries (LIBs) due to the limited nature abundance and regionally unbalanced reserves of lithium. Recently, sodium-ion batteries (SIBs) have been considered as one of the attractive next generation energy storage devices due to sufficient resources, low price, and similar electrochemical properties of sodium to those of lithium. However, because of the larger size and heavier atomic weight of sodium than lithium, graphite, the most common anode in LIBs, is difficult to be used in SIBs. Therefore, it is necessary to explore suitable high-performance anode materials for SIBs. Iron oxide (Fe_2O_3) has the merits as an anode material in SIBs due to the high theoretical capacity (about 1007.0 mA h g^{-1}), low cost, and non-toxicity. However, it suffered from severe volume changes during charge-discharge processes, mainly caused by the pulverization and agglomeration of Fe_2O_3 particles in the conversion reactions with sodium ions. Thus, low reversible capacity and cycle stability are frequently observed. To alleviate these problems, we synthesized Fe_2O_3 coated by N-doped graphitic carbon (Fe_2O_3/NGC) using dopamine as carbon and nitrogen sources. The Fe_2O_3/NGC composite shows enhanced electrochemical performances with an excellent reversible capacity of about 497.66 mA h g^{-1} at 100.7 mA g^{-1} after 150 cycles in the voltage range of 0.01-3.0 V, which value is significantly higher than those of the bare Fe_2O_3 sample.

Poster Presentation : **ELEC.P-417**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

FeF_2 Nanoparticles Embedded with Graphitic Carbon Derived from Fe-MIL-88B as a Cathode Material for Sodium-Ion Batteries

Achmad Yanuar Maulana, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

The concern about the scarcity of lithium in the future encourages the development of alternative rechargeable battery systems for lithium-ion batteries (LIBs). The beneficial factor of sodium such as low-cost material, high natural abundance, and similar electrochemical characteristic with lithium inflicted sodium-ion batteries (SIBs) as one of the most promising next-generation power sources. Iron difluoride (FeF_2) can be considered as one of suitable cathode materials to be applied in SIBs due to its high theoretical capacity (about 571 mAh g^{-1}), abundance, and low-cost main elements. However, the poor electrical conductivity of FeF_2 leads to insufficient reversible capacity and cycling stability in charge-discharge processes. In this work, FeF_2 nanoparticles were successfully embedded with graphitic carbon (FeF_2@GC) from Fe-MIL-88B, Fe-containing metal-organic framework, exhibiting a high discharge capacity of about 120.45 mAh g^{-1} at 50 mA g^{-1} after 300 cycles with good cycling stability.

Poster Presentation : **ELEC.P-418**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Electrochemical non-enzymatic glucose sensor based on nickel oxide with polydopamine

Tae-Won Seo, Hyewon Jang[1], Young Bong Choi[2], Hyug-Han Kim[2,*]

chemistry, Dankook university, Korea
[1]*chemistry department, Dankook University, Korea*
[2]*Department of Chemistry, Dankook University, Korea*

Glucose sensor has used enzyme to measure the concentration of glucose in the human blood. However, the glucose sensor has a problem with enzyme stability because the activity is changed according to various conditions such as pH, temperature and humidity. To solve this problem, the modified electrode measured glucose using nickel oxide without enzyme. The modified electrode was deposited more nickel oxide on the ITO/polydopamine(PDA) surface using functional group of PDA to form coordinate covalent bond with nickel oxide. We checked the electrode surface by using Electrochemical Impedance Spectroscopy (EIS), Field Emission Scanning Electron Microscope (FE-SEM) and Energy Dispersive X-ray Spectroscopy (EDX). Using cyclic voltammetry (CV), we confirmed the electrochemical reactions. As a result we studied that the modified electrode was shown possibility to use the glucose sensor.

Poster Presentation : **ELEC.P-419**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Pore size effects on the oxygen-involving electrocatalysis in truncated CoFe nanocubes

Sujin Jo, Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Porous nanomaterials can be synthesized following a number of chemical and physicochemical methods, such as hydrothermal, surfactant-based templating, sol-gel, and templated growth etc. According to the IUPAC classification, the pore size (diameter d) can be divided into three categories: micro- ($d < 2$ nm), meso- (2 nm $< d <$ 50 nm), and macroporous materials ($d > 50$ nm). Herein, we synthesized truncated CoFe nanocubes with two different pore sizes, i.e. mi-CoFe (average $d = 1.0$ nm) and me-CoFe (average $d = 31.5$ nm). The materials with tunable porosity are investigated as electrocatalysts for the oxygen evolution and oxygen reduction reactions (OER/ORR). The me-CoFe catalysts catalyzed the ORR via the efficient 4-electron process, whereas the mi-CoFe sample exhibited superior catalytic activity than the commercial Ir/C for OER. The electrocatalytic activity of the truncated CoFe nanocubes for oxygen-involving reactions in alkaline media was investigated by rotating disk electrode, rotating ring-disk electrode, and cyclic voltammetry. The compositional/structural features are characterized by high-resolution transmission electron microscopy, Brunauer-Emmett-Teller analysis, Fourier transform infrared and UV-Vis spectroscopy, X-ray photoelectron spectroscopy, and X-ray diffraction. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-420**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Insight into the role of a host-dopant in co-doping systems for efficient water splitting devices

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Doping engineering is of key importance for controlling the electrical, optical and structural properties of the semiconductor. Doping a naturally abundant hematite photocatalyst with heteroatoms is especially essential to boost its poor electrical properties for enhanced photocatalytic water splitting. For some impurities that create an unfavorable thermodynamic equilibrium, doped hematite with a reasonable photoelectrochemical performance needs to be synthesized under elaborate experimental conditions, which severely restricts the realization of hydrogen economy. To properly exploit cost competitive hematite as a photocatalyst for water splitting, it is crucial to seek an innovative doping strategy with thermodynamic equilibrium control. Here we show that the high formation energy of a Si-doped hematite can be decreased with the introduction of a host Ti-dopant via a thermodynamically favorable equilibrium process, making very easy and cost-efficient solution-based Si-doping possible.

Poster Presentation : **ELEC.P-421**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

A Hierarchically Structured Multi-dimensional Carbon Composite Anchored to Polymer Mat for Super-flexible Supercapacitor

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A carbon electrode was designed to guarantee flexibility of symmetric electric double layer capacitors (EDLCs) based on its architecture. Three different dimensional carbon materials were combined to achieve the flexibility without sacrificing high performances: highly capacitive but poorly-conductive three-dimensional graphene (3D-Gn*) as a platform for electric double layer formation, one-dimensional carbon nanotube (1D-CNT) as an electrically conductive highway and two dimensional graphene (2D-Gn) for facilitating electron communications between 3D-Gn* and 1D-CNT. From a mechanical standpoint, the 1D-CNT provided an intertangled framework to integrate the main active material 3D-Gn* and anchored the active layer to a flexible polymer matrix. Resultantly, the symmetric EDLC based on the hierarchically structured multi-dimensional carbon electrodes anchored to flexible substrates was operated successfully at 3 V, ensuring high energy densities even under repetitive mechanical stress conditions.

Poster Presentation : **ELEC.P-422**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Preparation and Electrochemical Investigation of TEMPOL Derivatives : Apply to Redox Flow Battery

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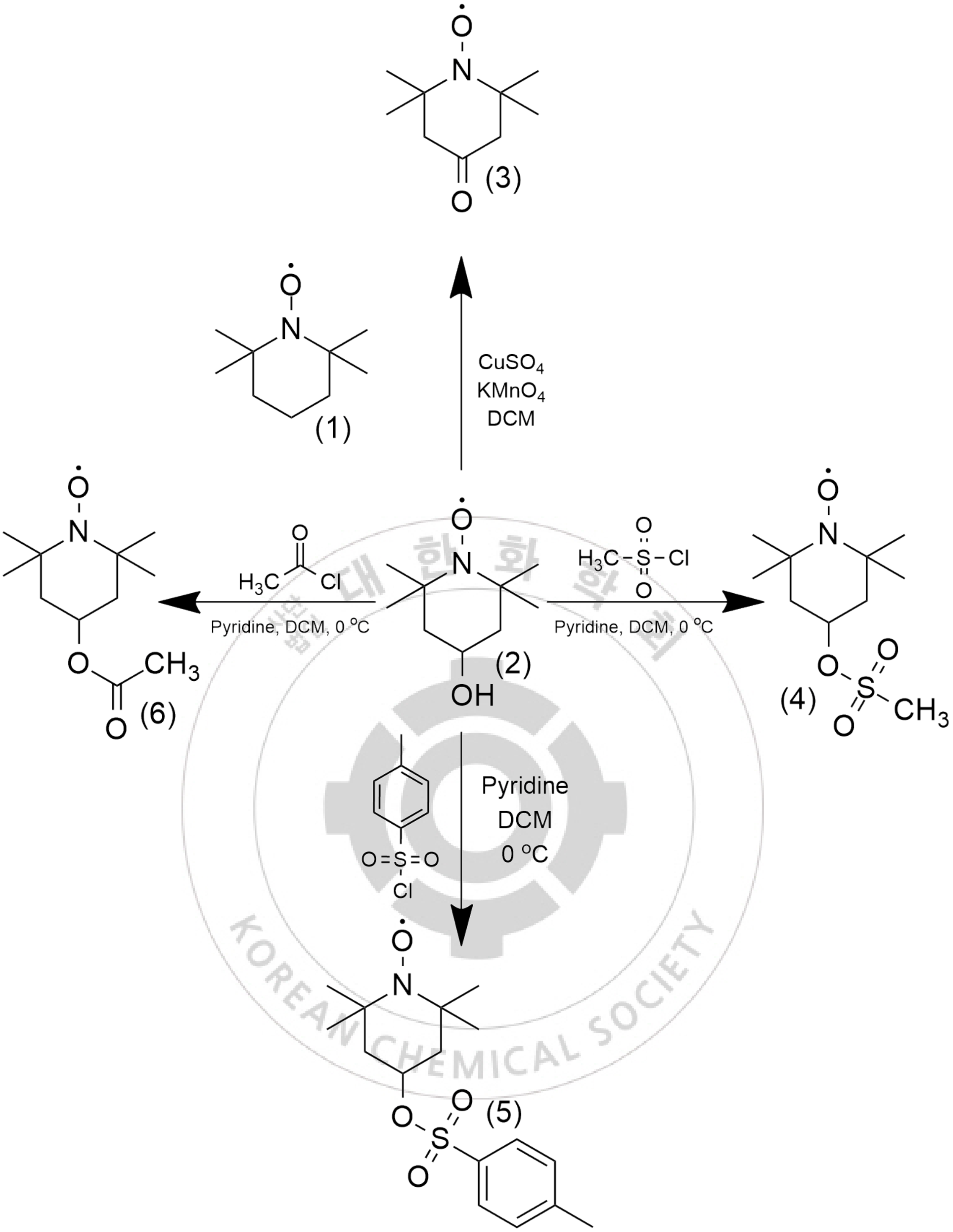
Recently TEMPO((2,2,6,6-Tetramethylpiperidin-1-yl)oxyl) is interesting organic catholyte in Redox Flow Batteries(RFBs) for offering the possibility of wide potential windows. Herein we report the investigation on relationship between electrochemical properties of TEMPOL(4-hydroxyl-TEMPO) derivatives. To do this we prepared TEMPOL derivatives and investigated CV results depending on their different functional group.


(3)
(1)
CuSO$_4$
KMnO$_4$
DCM
H_3C Cl
Pyridine, DCM, 0 °C
$H_3C-S-Cl$
Pyridine, DCM, 0 °C
(2)
OH
(6)
(4)
Pyridine
DCM
0 °C
O=S=O
Cl
(5)

Poster Presentation : **ELEC.P-423**

Electrochemistry

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Fe_2O_3 nanostructures for enhanced capacity of electrochemical capacitor

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We prepared α-Fe_2O_3 nanostructures assembled with nano-flakes formed through the decomposition of $Fe(CO)_5$ and interfacial growth of nano-flakes. The time-dependent flake growth was observed and their shape and characterization of materials were determined by SEM, TEM and XRD. AAO-templated iron tubes were also formed through the decomposition of $Fe(CO)_5$ and interfacial growth. The electrochemical behavior of iron nano-structured materials for electrode of capacitor was tested and compared over different sized nano-flakes, nanotubes, and conventional nanoparticles. Thus, α-Fe_2O_3 plates assembled with nano-flakes of 30 nm thickness gave an optimal result that specific capacitance was up to 171 Fg^{-1} and lowest capacitance decrease at high current density which showed better performance than conventional nanoparticles. These results imply that specific structure of α-Fe_2O_3 demonstrated by this work might be a solution which improves a performance from inherent low conducting problem. In addition, conducting polymer, polyaniline(PANI) could be composited with iron nano-structures to improve conductivity and capacity. In this work, the composited structures of PANI and iron nano-structures were demonstrated and their electrochemical behavior was investigated.

Poster Presentation : **ELEC.P-424**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Understanding reaction kinetics by tailoring metal co-catalysts of $BiVO_4$ photocatalyst

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In this study, the reaction mechanisms of metal-semiconductor composites used as photocatalysts were demonstrated by coupling the preparation of $BiVO_4$ with a consecutive photodeposition of metal nanoparticles. The photocatalytic activity of metal-$BiVO_4$ (M-$BiVO_4$, where M = Pt, Au, Ag) composites were evaluated through dye decomposition under UV-visible irradiation. The photocatalytic efficiency was significantly enhanced after Pt deposition compared to other M-$BiVO_4$ com-posites. The size or shape of $BiVO_4$ was not the main factor for efficiency of Pt-$BiVO_4$. However, deposited Pt co-catalyst was essential for the photocatalytic decomposition of dye on the $BiVO_4$ surface. Radical scavengers were employed to elu-cidate the reaction mechanism during photocatalytic reaction using Pt-$BiVO_4$ composite. This study provides details on the reaction mechanism of the photocatalytic reaction on a Pt at the $BiVO_4$ surface under solar irradiation.

Poster Presentation : **ELEC.P-425**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Solar energy conversion by cyanobacterium *Anabaena variabilis* using double mediators

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Photosynthesis taking place in the thylakoid membrane of plants, algae, and cyanobacteria is a highly developed system that uses solar energy. Recently, the whole photosynthetic organisms or units are being used as a photo-biocatalyst of photo-bioelectrochemical devices to convert solar energy to electrical energy. In this study, we suggest a method which converts solar energy into electric energy using cyanobacterium *Anabaena variabilis (A. variabilis)* with the 2,6-dimethyl-1,4-benzoquinone (DMBQ) and ferricyanide as an electron transfer mediator. Among several possible quinone derivatives, DMBQ was confirmed as a suitable lipid-soluble electron transfer mediator that accept electrons from cyanobacteria. In order to solve the low reversibility of DMBQ on the indium tin oxide (ITO) electrode surface, ferricyanide, which is reversible on the ITO electrode surface, was employed as the complementary mediator to transfer the electrons of $DMBQH_2$ to the electrode. When two mediators were used, the photocurrents generated from A. variabilis were observed. The photocurrent more than 2 mA cm^{-2} was observed at 60 μg Chl mL^{-1} of *A. variabilis* containing double mediators under one sun irradiation. This result shows possibility of converting solar energy to electricity using photosynthetic microorganisms as a photo-biocatalyst for water oxidation.

Poster Presentation : **ELEC.P-426**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Photoelectrochemical Coulometric Sensing of *Anabaena variabilis* Through a Mediated Electron Transfer System

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It is a worthwhile issue to predict the population of cyanobacteria to prevent algal bloom. Unlike existing methods for detecting cell population such as direct cell enumeration or fluorescence measurement, we developed a simple and fast coulometric system to detect the reduced redox mediator from electrons generated by photosynthesis of cyanobacteria. 2,6-dimethyl-1,4-benzoquinone (DMBQ) is a suitable redox mediator in this system in that it can diffuse in and out of the cell membrane to reach to the thylakoid membrane and has a proper formal potential to harvest electrons, which can pass through electron transport pathway embedded in the thylakoid membrane. The red light, wavelength of 660 nm, was used to prevent a reduction of DMBQ itself by light without cyanobacteria. To identify the electron flows from a low concentration of cyanobacteria, glassy carbon rod, which is a highly sensitive material was applied. The detecting limitation point of 2.45 mg L^{-1}, which is corresponding to 3.5×10^8 cells mL^{-1} was identified from this system, and this has never been reported. The results show a simple and fast detectable coulometric cyanobacterial sensor that can identify the generated electrons from photosynthesis electrochemically. Also, it shows the possibility of a real-time monitoring amperometric sensor through the further improvement of the system.

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Poster Presentation : **ELEC.P-427**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Comparing activity of δ-MnO2 with various intercalated cation toward alkaline oxygen evolution reaction

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

Hydrogen economy has got attention as renewable energy system. To produce hydrogen without the emission of carbon dioxide, water splitting intergrated solar cell is one of solution. However, high overpotential in anode and high price of catalyst inhibits its commercialization of water splitting. Manganese oxides have various redox chemistry and are thus advantage for energy storage and conversion due to its high surface area and abundance. According to recent in situ XAS results, Mn oxide turns to δ-MnO2 at 1.45 VRHE and retains their structure during OER. δ-MnO2, which is octahedral MnO6-layered structure with cations and water intercalatered into interlayer structure, has an oxidation state between III and IV and are a candidates of active phase for OER. In this study, we synthesized Birnessite-like Mn oxide with metal cations with facile sol-gel method. We also compared their OER activity in neutral and alkaline electrolyte and investigated on the role of metal cation in the oxidation state of Mn oxide.

Poster Presentation : **ELEC.P-428**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Quantitative analysis of electrochemically generated polyiodides (I_{2n+1}^-, n = 1 - 3) in acidic media by electrochemical titration on Pt ultramicroelectrode

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Department of Chemistry, Hanyang University, Korea

Polyiodides-speciation from electro-oxidation of I^- on an electrode in an aqueous solution with highly concentrated ZnI_2 media has been barely understood. It has been reported that I_3^- is the main polyiodide species in an aqueous solution due to instability of higher orders of polyiodides, such as I_5^- and I_7^-. In this study, we analyze polyiodides speciation existing at an electrode surface during electro-oxidation of I^- at steady state through the voltammetric titration of I_2 film by I^-. In this case, i_{ss} would be mainly proportional to concentration of free I^-, which is equilibrated with surface-precipitated $I_{2(s)}$ to form either I_3^- or higher orders of polyiodides. Furthermore, we also present the more rational mechanism for formation of I_2 film at steady state than previous studies such as a formation of a porous I_2 film at steady state or formation of I_2 film with a certain amount of I^- to maintain a film conductivity.

Poster Presentation : **ELEC.P-429**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Viologen-bromide dual-redox ionic solid complexes: understanding their electrochemical formation and redox-chemistry via proton-coupled electron transfer (PCET)

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Inhibition of self-discharge in a redox-enhanced electrochemical capacitor (Redox-EC) is crucial for excellent energy retention. Heptyl viologen dibromide ($HVBr_2$) was chosen as a strong candidate as a dual-redox species due to its solid complexations in the electro-oxidation of Br^- to form $[HV^{2+}\cdot 2Br_3^-]$ and electro-reduction of HV^{2+} to render $[HV^{+\cdot}\cdot Br^-]$. In this article, we present detailed electrochemical studies of formation of $[HV^{2+}\cdot 2Br_3^-]$ and $[HV^{+\cdot}\cdot Br^-]$, their redox features, and galvanic exchange reactions between the two types of dual-redox ionic solids on Pt ultramicroelectrode (UME) in neutral (0.33 M Na_2SO_4) and acidic (1 M H_2SO_4) solutions. Most importantly, through voltammetric and particle-impact electrochemical analyses, we found that the redox and galvanic exchange reactions of the two dual-redox ionic solid complexes occur via proton-coupled electron transfers (PCETs), and H^+ transfer is the key process to limit the over-all kinetics of the electrochemical reactions. We also rationalize the galvanic exchange reaction via PCET based on computational simulation.

Poster Presentation : **ELEC.P-430**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Stochastic electrochemical cytometry of human platelets via particle collision approach

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The quantitative analyses of human platelets are important for the diagnosis of various hematologic and cardiovascular diseases. In this article, we present stochastic particle impact electrochemical (SPIE) approach for human platelets with the fixation (F-HPs), and, for achieving the standard platform of SPIE-F-HPs, carboxylate functionalized polystyrene particles (PSPs) are studied as well.For SPIE-PSPs (or F-HPs), $Fe(CN)_6^{4-}$ was used as the redox mediator, and electro-oxidation of $Fe(CN)_6^{4-}$ to $Fe(CN)_6^{3-}$ is derived on a Pt ultramicroelectrode (UME) by applying the constant potential, where the corresponding oxidation current is mass-transfer controlled. When PSPs (or F-HPs) are introduced to an aqueous solution with $Fe(CN)_6^{4-}$, sudden current drops (SCDs) were monitored, which result from partial blockage of a Pt UME by collision of an individual PSP (or F-HP). For SPIE-PSPs (or F-HPs), we found that it is essential to enhance migration of mass-transfer for PSPs (F-HPs) toward a Pt UME by maximizing steady state current associated with electro-oxidation of $Fe(CN)_6^{4-}$, resulting from increasing its concentration to the solubility limit. We successfully measured concentration of F-HPs dispersed in an aqueous solution containing $Fe(CN)_6^{4-}$ with minimum detectable concentration of 0.1 fM, and the size distribution of F-HPs is also estimated from the obtained idrop distribution based on the SPIE analysis, where idrop stands for magnitude of current drop of each SCD. Lastly, it is revealed that HPs without the fixation process (WF-HPs) is difficult to be quantitatively analyzed by SPIE because of their transient activation process, which results in the change of their spherical shape. The observed difficulty is also supported by finite element analysis, which shows that idrop can be significantly increased as an elongated WF-HP is adsorbed on an edge of an UME.

Poster Presentation : **ELEC.P-431**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Time Transient Electrochemical Monitoring of Tetraalkylammonium Polybromide Solid Particle Formation: Observation of Ionic Liquidto-Solid Transitions

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Energy storage systems (ESSs) using a Br^-/Br_2 redox reaction such as a Zn/Br redox flow battery (RFB) or a redox-enhanced electrochemical capacitor (Redox-EC) suffer from self-discharge reactions resulting in significant coulombic loss. To inhibit the self-discharge, quaternary ammonium (Q^+) and tetraalkylammonium (T^+) bromide are added to form ionic liquid (QBr_{2n+1}) and solid (TBr_3) polybromides during the ESS charging process. The electrochemical formation of liquid QBr_{2n+1} and its electrochemical properties have been examined. The detailed mechanisms of ionic solid TBr_3 formation, however, have not yet been explored. In this article, we analyzed the ionic liquid-to-solid phase transition of TBr_3 particles using a time transient electrochemical method. We suggest the formation of ionic solid TBr_3 particles via hydrated TBr_3 droplets as an intermediate phase, which are generated by electro-oxidation of Br^- in an aqueous TBr solution. We found the phase transition time of TBr_3 particles is strongly dependent on the chemical structure of T^+ and the concentration of TBr in an aqueous solution.

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Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Synthesis, Characterization and Photoelectrochemical Properties of Green Route Deposited Iron Vanadate Thin Films

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Photoelectrochemical (PEC) water splitting is an attractive and sustainable approach to produce the clean energy. Iron vanadate (FeVO4) is emerging as novel and promising n-type multi-metal oxide semiconductor for PEC water splitting. Herein, the synthesis of FeVO4 thin films via facile successive ionic layer adsorption and reaction (SILAR) route have been reported. The synthesized thin films were characterized for their structural, surface morphological, optical, photo electrochemical and charge transport properties. X-ray diffraction patterns confirms the formation of pure anorthic phase of FeVO4 after annealing at 550 0C. The FE-SEM micrographs show the formation of the dense array of FeVO4 grains. EDAX result reveals the high purity of FeVO4 composition. The optical band gap values about 2.06 eV reveals the broader visible light absorption. Also, the detailed PEC properties have been elaborated.

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Poster Presentation : **ELEC.P-433**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Facile Synthesis of $Ni(OH)_2$ Decorated Pt-Cu Octahedra and Their Electrocatalytic Activity toward Ethanol Oxidation Reaction

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Nanoscale electrocatalysts for ethanol oxidation reaction (EOR) applying to direct ethanol fuel cell as alternative energy system have been actively studied. Here we report the synthesis of 9 nm $Ni(OH)_2$ decorated Pt-Cu octahedra ($Ni(OH)_2$-PtCu) in one-pot synthesis for EOR electrocatalysis in acidic electrolyte. To synthesize $Ni(OH)_2$-PtCu octahedra, CO gas was directly introduced in a reaction process as selective capping agents on the Pt-Cu(111) facet. $Ni(OH)_2$ was naturally deposited on the Pt-Cu octahedra during the synthesis. Carbon supported $Ni(OH)_2$-PtCu ($Ni(OH)_2$-PtCu/C) as an EOR catalyst showed enhanced CO tolerance due to the existence for oxophilic $Ni(OH)_2$ on the surface of Pt-Cu, facilitating water dissociation to produce OH adsorption and to promote complete CO oxidation to CO_2. Therefore, the $Ni(OH)_2$-PtCu/C showed enhanced EOR activity and durability compared to the Pt-Cu octahedra and commercial Pt/C counterparts.

Poster Presentation : **ELEC.P-434**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Wiring system for direct electron transfer between electro-inactive bacteria and electrodes using modified carbon nanoparticles

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Direct electron transfer (DET) from bacteria to electrodes is one of the key factors to improve the power density of microbial fuel cells (MFCs). Since microorganisms that can perform extracellular electrons transfer are generally anaerobic bacteria and few in number, it is very important to construct MFCs with aerobic and electrochemically inactive bacteria. However, conductive wiring systems are required for electron transfer between the electro-inactive bacteria and the electrodes. Here we report how we partly succeeded in direct electron transfer from *Escherichia coli (E.coli)* using carbon nanoparticles (CNPs) as an electron conduit. To improve accessibility of CNPs to the inner membrane of *E. coli*, CNPs were modified with 4-aminophenyl groups (4AP). Thus, modified 4AP-CNPs have hydrophilic properties and positively charged that induces electrostatic interaction with negative charges of the microbial outer membrane to form a 4AP-CNPs/*E. coli* complex. In addition, the carbon cloth (CC) electrode was modified with 4-carboxylphenyl group (4-CP) to improve the contact between 4AP-CNPs/*E.coli* and electrodes. The direct electron transfer was confirmed by cyclic voltammetry using glucose as substrate. Glucose oxidation was observed -0.15 V vs. Ag/AgCl, indicating electrons produced from glucose oxidation were captured by CNPs and transferred to the electrode. Oxidation current tends to increase with glucose concentration. Without *E. coli*, no oxidation current was observed. This work shows the possibility of direct electron transfer even from electrochemically inactive bacteria.

Poster Presentation : **ELEC.P-435**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Highly Graphitized Carbon for Oxygen and Nitrogen Electrochemistry

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Proton exchange membrane fuel cells (PEMFCs) have been developed and partially commercialized in fuel cell vehicle and stationary field. However, there still remain technical issues especially in the cathode part where an oxygen reduction reaction (ORR) occurs. The large overpotential of the sluggish ORR and the water management issues dramatically affect the performance of a membrane electrode assembly (MEA) in PEMFCs. Additionally, the durability of MEAs is also a key issue for the further development of PEMFCs.Ammonia is regarded as a potential energy carrier because of its' high volumetric energy density and easier transportation/storage. Ammonia electrooxidation, which is the anodic reaction of ammonia electrolysis, has been investigated mostly on platinum (Pt) or iridium (Ir) catalysts. Due to the sluggish kinetics of ammonia elelctrooxidation reaction (AOR), it is required to design and develop more active catalysts for AOR. For achieving the high activity of catalysts for AOR, it is also important to understand the reaction kinetics and poisoning mechanism.In this study, highly graphitized carbon has been synthesized and used as a support material for ORR and AOR. Due to the unique pore structure and surface properties of highly graphitized carbon, the performance and durability of oxygen and nitrogen electrocatalytic reactions have been greatly improved.Reference[1] S. Chung et al. J. Power Sources, 399, 350-356 (2018);[2] J. Gwak et al. ChemSusChem, 9, 403-408 (2016).

Poster Presentation : **ELEC.P-436**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Fabrication g-C_3N_4@SnO_2 for Photoelectrochemical watersplitting

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The g-C_3N_4 is easily synthesized by annealing the melamine. The electronic band gap of 2.7eV can promote the absorption toward the visible light. Compare with SnO_2 nanoplates, g-C_3N_4@SnO_2 was more enhance photocurrent density. In this research, 1-dimensional SnO_2 nanoplates was fabricated on the FTO glass by the hydrothemal treatment and post-thermal treatment. The g-C_3N_4 was synthesized by annealing the melamine powder. After grinding, g-C_3N_4 powder was dispersed in isopropanol and sonicated and filtered. Finally, g-C_3N_4@SnO_2 was fabricated by electrophoretic deposition. More detail analyses such as FE-SEM, XRD, UV-VIS and PEC performance would be presented.

Poster Presentation : **ELEC.P-437**

Electrochemistry

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Overestimation of photoelectrochemical hydrogen evolution reactivity induced by noble metal impurities dissolved from counter/reference electrodes

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Photoelectrochemical (PEC) hydrogen production by solar-driven water splitting is a promising and environmentally benign methods to convert solar radiation into a fuel. However, low stability and efficiency of photocathode have been the issue for solar-hydrogen conversion efficiency in water splitting reactions. HER activity and long-term durability are the two most important parameters for the evaluation of their success in the PEC systems. In general, these experimental conditions are assessed using conventional three-electrode system comprising of working, counter and reference electrodes in a batch cell configuration. Pt counter electrode is commonly used due to its high activity and stability in electrochemical reactions. However, Pt dissolution during the electrochemical operations have been observed by in situ inductively coupled plasma-mass spectrometry (ICP-MS) under potentiodynamic conditions. Concurrently, redeposition of Pt ions have been known to influence the activity of the working electrode. In this work, we have investigated the validity of conventional three-electrode system employed with Pt counter and Ag/AgCl reference electrodes for evaluation of PEC cathodes. With a model cathode of p-Si, significant overestimation of the experimental parameters was found during and after the general voltammetric protocols of PEC measurements. Potential variations on the Pt counter electrode were concurrently monitored during the PEC evaluations, of which results were coupled to in situ ICP-MS analysis to simultaneously quantify its dissolution. Post-reaction spectroscopic/microscopic measurements confirmed redeposition of Pt. Interestingly, Ag in the form of metallic state was confirmed on the surface of p-Si, indicating the possible interference during the HER

Poster Presentation : **ELEC.P-438**

Electrochemistry

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Flexible TiO2 nanotubes/Ti mesh electrodes for carbon dioxide reduction

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A manned spacecraft environmental control and life support system (ECLSS) is a group of systems that allow human to live in space for long term exploration. Thus, designs and developments are critical for human health and successive space mission. Generally ECLSS consists of several main components such as, atmosphere revitalizations (CO2 removal/reduction, O2 generation/supply, trace contaminant monitoring and control, microorganism control), water recovery and managements (water storage & distribution, water recovery, water quality monitoring). Many studies of water/air purifications and decompositions of contaminant/microorganisms using TiO2. Conventionally, powdered TiO2 is used, which limits the photocatalytic activity because of small surface area. Thus, developments and applications of nano-sized TiO2 structures, such as nanotubes and nanorods are advantageous. In this study flexible TiO2 nanotubes/Ti mesh were prepared and tested for different parts of the ECLSS. In first step photocatalytic oxygen generation using TiO2 nanotubes/Ti mesh will be performed. In second and third step CO2 photoreduction and water purification systems using TiO2 nanotubes/Ti mesh will be developed and tested, respectively. In fourth step, air purification systems will be developed. In final step TiO2 nanotubes/Ti mesh in cylinder type reactor will be employed to develop anti-contaminant and antibacterial systems.

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Double walled TiO2 nanotubes for photo-catalytic CO2 reduction

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[1]*Department of Advanced Materials Engineering, Kumoh National Institute of Technology, Korea*

We have studied several methods such as dip-coating, spin-coating and electro-deposition to deposit double walled TiO2 nanotubes on mesoporous media. From the preliminary morphological and photo-current studies, electro-deposition was found to be the appropriate method for the deposition of double walled TiO2 nanotubes. We then systematically investigated to obtain the optimum condition for improved photo-electrochemical properties by changing various factors like time, concentration, voltage, annealing temperature and media. Sensitized double walled TiO2 nanotubes have shown superior activity under visible light irradiation and large reactive surface area. Finally, but most importantly efficiency of double walled TiO2 nanotubes on mesoporous media were comparatively studied by photo-induced CO2 reduction test.

Poster Presentation : **ELEC.P-440**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Electrical property of epoxy resin-double walled TiO2 nanotubes composites

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Epoxy resins have been applied to coatings, electronic devices, and adhesives for improved TiO2 composites because of their outstanding tensile strength, adhesion strength, heat transfer resistance, and electrical resistance. The properties of cured epoxy resins are influenced by the kind of epoxy resin, curing agent, and curing method. This epoxy resin-double walled TiO2 nanotubes composite is characterized using photo-electro-catalytic CO2 reduction reaction. The sun light assisted conversion of CO2 into small organic molecules is emerging and seriously considered, over the world, as a valuable eco-friendly route for CO2 treatment. TiO2 is recognized for its highly economical advantage, its chemical stability and its photo-active properties. It is a photocatalytic materials which, under certain conditions, like a coupling with a conductive graphene sheet, may produce highly valuable chemical products such as formic acid, methanol and methane by redox photo-conversion of CO2. Among various CO2 reduction products, methanol can be an alternative of gasoline. It can be also used as a cheap chemical reagent for the production of ethylene, propylene or more complex molecules in chemical industry. Finally, it can be used in fuel cells instead of hydrogen, reducing the dependency of this energy technology to liquefied fossil natural gas. It is expected that solar light-assisted CO2 conversion in methanol will be increasingly significant as a solution for environmental problems, allowing the development of green economies and opening business opportunities. (Young Baek Kim as second author of this abstract contributed to epoxy resin preparation, affilation: IPTEC CO.,LTD, 3, Seongseogongdanbuk-ro, Dalseo-gu, Daegu, Republic of Korea)

Poster Presentation : **ELEC.P-441**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Large-scale synthesis of high-quality carbon nanoparticles and their electrocatalytic performance

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Carbon nanoparticles (CNs), also known as carbon dots, have been recognized as sp^2 conjugated and quasispherical particles with sizes below 10 nm. They generally contain suitable oxygen-containing species such as carboxyl, hydroxyl, and aldehyde groups. Herein, direct synthesis of CNs in a controllable manner was achieved using hydrogen peroxide at atmospheric pressure conditions. The synthesis is accomplished via a single step using ethylene glycol and ethanolamine (or ethylenediamine) as carbon and nitrogen precursors. On the other hand, the conductivity and surface properties of CNs are key properties affecting the electrocatalytic performance. These properties of CNs depend strongly on the fabrication methods. To obtain highly active nanostructures, we fabricated all-carbon hybrid nanocomposites, i.e. carbon nanotube (CNT) decorated by CNs (CNT-CNs), via hydrothermal synthesis. The synthesized CNs and CNT-CNs were characterized by UV-Vis absorption, photoluminescence spectroscopy (PL), infrared (IR), X-ray photoelectron spectroscopy (XPS), AFM microscopy and high-resolution TEM (HR-TEM). The CNs and CNT-CNs obtained were also investigated for their influence on the electrocatalytic benefits. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-442**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Enhanced Catalytic Activity of SOx-Incorporated Graphene for Hydrogen Evolution Reaction

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The intrinsic catalytic activity of carbon-based nanostructures can be improved by incorporating heteroatom defects that result from geometric and electronic effects. Therefore, sulfur defects are used to enhance the catalytic activity of carbon-based nanostructures in hydrogen evolution reaction (HER). This is accomplished by increasing the hydrogen adsorption ability due to the large size of sulfur atoms, which induces structural deformation by increasing the sp3 character of graphene carbons. However, the effect of sulfur oxidation on HER catalytic activity has not yet been discussed, even though sulfur can easily be oxidized to sulfur oxide (SOx) in acidic environments, which may decrease the metallicity of graphene by opening the bandgap. Herein, we systematically investigate the HER catalytic activity of SOx-incorporated graphene, SOx@G (x=2, 3 or 4), based on the electronic, thermodynamic and kinetic viewpoints. Our results reveal that SO3@G on the basal plane has superior HER catalytic activity among the SOx@G materials due to its metallic nature and ability to stabilize adsorbed hydrogen (H*) that results from electrostatic interactions between SO3 and H* in an intermediate state. As a thermodynamic descriptor of the HER catalytic activity, the hydrogen binding Gibbs free energy (ΔG^{Volmer}) is calculated as -0.04 eV for SO3@G in the Volmer step, which is the most improved value. In particular, this value is close to zero, making SO3@G the ideal catalyst compared to S@G. In addition, the activation energies at both the Volmer and Tafel steps (ΔE^{Volmer} and ΔE^{Tafel}, respectively) of SO3@G show the lowest energy barriers among SOx@G, taking values of 0.005 eV and 0.14 eV, respectively. Thus, these values can be used as kinetic descriptors that are close to that of conventional Pt catalysts.

Poster Presentation : **ELEC.P-443**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Comparing Activity of S-doped Carbon Nanofiber depending on C-S bond toward Alkaline Oxygen Reduction Reaction

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Fuel cell technologies have attracted due to their various advantages, such as high power density, and low working temperature. However, some limitations still remain, such as sluggish kinetics of oxygen reduction reaction (ORR) and the high price of Pt, one of the most active catalysts in both anode and cathode. Thus metal-free catalyst based on carbon materials has attention. the S atom can change the spin density in the carbon π-system, which can further promote the catalytic activity of the ORR. However, S atom and some C-S bond are known as a non-active site for ORR, while they cause 2 electron reaction, hydrogen peroxide production. In this study, we synthesized carbon nanofiber via electrospinning and impregnated S atoms in the carbon nanofiber by successive heat treatment. The kinds of C-S bond on S-doped carbon nanofiber were dependent on the heat treatment temperature. It caused different activity trend of ORR or hydrogen peroxide production in alkaline media. Thus we investigated the number of a participated electron during reduction using a rotating ring disk electrode method and figured out the relationship between the activity and kinds of C-S bond confirmed by XPS and TGA.

Poster Presentation : **ELEC.P-444**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Metal-Free Heteroatom (B, N)-doped Carbon as Bi-functional oxygen catalyst for Zinc-Air Battery

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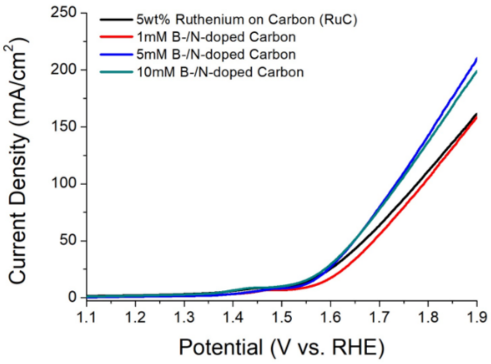
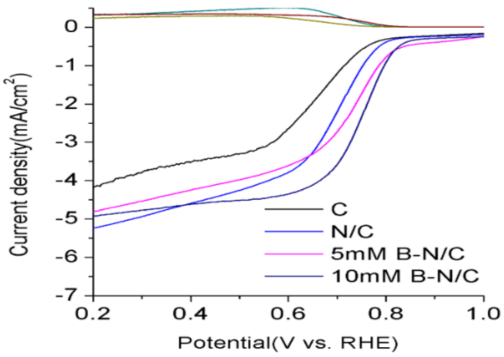
Rechargeable zinc-air battery is one of the powerful candidates for future energy storage system due to its simple structure, safe application, and high theoretical specific capacity. However, due to its high cost and low durability of commercial noble metal catalyst, the zinc-air battery is still not in wide application to various fields. For this reason, many noble metal-free catalysts, such as Heteroatom-doped carbon is attracting much attention by its economical aspect and competitable catalytic performance. When dopant is added to the carbon matrix, electrochemical catalytic performance is increased due to the activity sites induced from different electronegativity between dopant and carbon. However, since each dopant affects different to catalytic performances, it is important to discover the effect of each dopant and synergetic effect between each dopant. So, in this study, we applied plasma bottom-up synthesis as a simple and fast carbon-based heteroatom-doped catalyst. Quinoline (C9H7N) as the nitrogen(N) dopant precursor and boric acid(H3BO3) as the Boron(B) dopant precursor was applied. Further, to investigate synergetic effect of boron and nitrogen, boric acid was applied 1mM to 10mM to nitrogen precursor. In the electrochemical analysis, 10mM B-N doped Carbon showed best ORR onset potential (0.86V vs. RHE), which is higher than that of 1mM B-N doped Carbon and 5mM B-N doped carbon (Figure 1). Also, to applying rechargeable Zn-Air battery system, OER performance is investigated and as a result, 10mM B-N doped carbon showed highest OER performance (1.5V vs. RHE, Figure 2). Based on the results, we can suggest that synergetic effect of Boron and Nitrogen can be used for the new approach to replace noble metal-based


5wt% Ruthenium on Carbon (RuC)
1mM B-/N-doped Carbon
5mM B-/N-doped Carbon
10mM B-/N-doped Carbon
Current Density (mA/cm^2)
250
200
150
100
50
0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
Potential (V vs. RHE)


Current density(mA/cm^2)
0
-1
-2
-3
-4
-5
-6
-7
C
N/C
5mM B-N/C
10mM B-N/C
0.2
0.4
0.6
0.8
1.0
Potential(V vs. RHE)

Poster Presentation : **ELEC.P-445**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Red Phosphorescent Phenylisoquinoline-based Iridium(III) Complexes using for Solution-Processed Organic Light-Emitting Diodes

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Red phosphorescent iridium(III) complexes, (TPIQ)$_2$Ir(acac) and (TPIQ)$_2$Ir(ppy), based on 1-(4-(trimethylsilyl)phenyl)isoquinoline (TPIQ) as the cyclometalated main ligand and either acetylacetone (acac) or 2-phenylpyridine (ppy) as an ancillary ligands, were synthesized for solution-processed organic light-emitting diodes (OLEDs). The Ir(III) complex, (PIQ)$_2$Ir(acac), which consists of 1-phenylisoquinoline (PIQ) as the main ligand and acac as the ancillary ligand, was also synthesized as a reference. The photophysical, electrochemical, and electroluminescent (EL) properties of Iridium(III) complexes were investigated. Red OLED using (TPIQ)$_2$Ir(ppy) as an emitter exhibited significantly more improved a full-width at half-maximum (FWHM) by introduction of ppy as an ancillary ligands. The EL spectrum of (TPIQ)$_2$Ir(ppy) exhibited emission maximum at 640 nm with a full-width at half-maximum (FWHM) of 113 nm and Commission Internationale de L'Eclairage (CIE) coordinates of (0.68, 0.32) at 1000 cd/m^2. The device with 7 wt% doping concentration of (TPIQ)2Ir(ppy) exhibited maximum luminance of 6,296 cd/m^2, maximum luminous efficiency of 15.93 cd/A, power efficiency of 5.26 lm/W, and external quantum efficiency of 5.45 %, respectively.

Poster Presentation : **ELEC.P-446**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Addition of Ultra-thin Au Layer underneath Mn oxide for Alkaline Oxygen Evolution Reaction

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The overpotential in the anode, happens oxygen evolution reaction (OER), contributes much more to the voltage drop during electrolysis than that in the cathode. Hence, substantial effort has continuously been devoted to finding the most effective catalyst metal/metal oxide for oxygen evolution reaction based on mainly Ni, Co, Fe and Mn in especially alkaline media OER. However, Mn showed lower activity compared to Co and Ni as the catalytic metal ion. During OER, four electrons are produced and they should be transferred for the facilitated reaction. Since Au is the highest electronegativity among metal, OER on Mn oxide on the Au layer can be enhanced by taking a produced electron from Mn to Au and maintaining Mn active oxidation state. In this study, we synthesized an ultra-thin Au layer on a carbon electrode via sputtering and loaded Mn oxide catalyst on the Au electrode. The thickness of the Au layer was controlled by the sputtering time and confirmed by cross-sectional scanning electron microscopy. We investigated the OER activity depending on the thickness of Au by electrochemical test and the role of Au layer by comparing electron structure of Au and Mn before and after OER test.

Poster Presentation : **ELEC.P-447**
Electrochemistry
Exhibition Hall 1, THU 11:00~12:30

Label-Free Electrochemical Detection of Protein Kinase A Activity with C-Kemptide-AuNP/rGO-GCE

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Protein kinase A (PKA), playing a key role in the human biological system, especially involving in peptide phosphorylation and enzymatic signal amplification. PKA activity provides many information of some disease, such as cancer, leukaemia, HIV. Therefore, a lot of researchers have developed various methods to detect the activity of PKA sensitively and selectively. Here, we designed the label-free method to selectively detect the PKA activity with electrochemical impedance spectroscopy (EIS). The electrode for the EIS measurements was modified with gold nanoparticle/reduced graphene oxide (AuNP/rGO) hybrid nanocomposite to enhance the electrochemical catalytic effect. The AuNP/rGO hybrid nanocomposite was fabricated by simple and environmentally friendly method using electrochemical technique. For the PKA activity detection, the C-Kemptide was immobilized onto AuNP/rGO modified electrode (KAG-GCE) through gold-thiol bond. As-prepared KAG-GCE was characterized by scanning electron microscopy (SEM), cyclic voltammetry (CV), and EIS. Here, the Rct in EIS measurement was representing the change in PKA activity; the Rct increased with phosphorylation of C-Kemptide by PKA. So, we measured the PKA activity though changes in Rct according to the concentration of ATP and PKA. The inhibition assay was also performed with the H-89 kinase inhibitor. Furthermore, the KAG-GCE based PKA assay was applied to the ovarian cancer cell lysate. Our PKA assay showed a great potential for the use of actual clinical diagnosis.

Poster Presentation : **ELEC.P-448**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Electrochemical Aptasensor for Detection of Pb^{2+}-using Methylene Blue Tagged DNA and ERGO

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We have developed a sensitive aptasensor for the detection of Pb^{2+} ions based on G-quadruplex DNA and an electrochemically reduced graphene oxide (ERGO). Here, ERGO was coated on a glassy carbon electrode (GCE) surface by reduction of graphene oxide using cyclic voltammetry. After that, a methylene blue (MB)-tagged, guanine rich DNA aptamer (Apt) was attached on ERGO surface via π- π interaction. In the presence of Pb^{2+}, Apt forms G-quadruplex, leading to the detachment of Apt from the surface of ERGO/GCE. So the conformational change caused by Pb^{2+} produces the change in electrochemical signal. Electrochemical measurements showed highly sensitive detection of Pb^{2+} ions with a liner range from 10^{-15}~10^{-9} M and a detection limit of 0.51 fM. The sensor also has high selectivity of Pb^{2+} ions, high stability, reproducibility, and regeneration.

Poster Presentation : **ELEC.P-449**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

Ultrasensitive electrochemical aptasensor for Hg2+ using DNA coated reduced graphene oxide electrode

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

A highly sensitive electrochemical sensor was developed for the detection of Hg2+ ions in aqueous solution using a thymine (T)-rich aptamer and reduced graphene oxide (RGO) modified electrode. The method used methylene blue (MB) tagged aptamer which characteristic of electrochemical signal indicator. ERGO was synthesized and deposited on a glassy carbon electrode to enhance the electrode's conductivity, surface and conjugate the MB tagged aptamer by π-π interaction. In the presence of Hg2+, the MB tagged aptamer on the RGO modified electrode builds a hairpin structure which results in its subsequent detachment from the RGO surface. This conformational change causes significant decrease in voltammetric signals. We demonstrated that this sensing strategy showed high sensitivity and selectivity for Hg2+ detection. The fabricated aptasensor showed a linear detection range of 1 fM to 100 nM and detection limits of 0.16 fM for Hg2+. This aptasensor could be regenerated using cysteine.

Poster Presentation : **ELEC.P-450**

Electrochemistry

Exhibition Hall 1, THU 11:00~12:30

The few-layer graphene produced by urea-assisted liquid phase exfoliation of graphite

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Abstract. In this paper, we developed the method of mass production of few-layer graphene of high quality with low defect using direct shear mixing methods among mechanical exfoliation methods. We also enhanced the effect of exfoliation in water solution by using the inorganic salts urea and effectively achieved exfoliation by re-dispersion the graphene one of the organic solvents N-methyl-2-pyrrolidone (NMP). At this time, the urea acts not only as an assistant material, but also as a stabilizer to help the graphene in water to be dispersed. In this experiment, we found optimal conditions by changing the parameters: mixing time, shearing speed, urea concentration to maximize the concentration, defect, layers of graphene. Graphene produced under these optimal conditions was characterized through UV-vis spectra, Raman spectroscopy, TEM, SEM, and XPS using only the supernatant obtained from the process of centrifugation of 3000 rpm, 15 min. This confirmed that graphene produced through the method presented in this paper produced graphene sheets of high quality of few-layer graphene.

Poster Presentation : **EDU.P-459**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Exploring the Variation and Relationship with Actual Practice of Meta-Modeling Knowledge(MMK) Progression Levels for the Science Gifted

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[2]*Department of Chemical Education, Korea National University of Education, Korea*

The purpose of this study is to investigate the variation and the relationship between actual practice of MMK progression level for the science gifted. First, the Rasch model was used to measure MMK progression level of 51 students twice during the interval of one year. Thereafter, chi-squared test was used to determine whether there was a significant change in MMK progression level. As a result of chi-squared test, there was no statistically significant change in MMK progression level($p>.05$). Secondly, we analyzed the relationship between MMK progression level and practice for 7 gifted students. As a result of the analysis, it was confirmed that the student's response in practice can not exceed MMK progression level. There were also cases where students have high MMK progression level showed low response in practice. The results of these two studies show that gifted education programs are needed to increase MMK progression level and to provide gifted education that can connect knowledge and practice.

Poster Presentation : **EDU.P-460**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

The Effects and Changes that Argument-based Inquiry Activities Have upon the Claim-Evidence of Scientific Writings by Elementary School Students

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Department of Chemical Education, Pusan National University, Korea

This study investigated how argument-based inquiry activities influence and change the claim-evidence of elementary school students' scientific writings. In order to do so, for two classes of 33 fifth grade students, argumentation programs had been applied to 5 topics for one class of experiment group consisting of 17 students, while the activities suggested in textbooks had been utilized for the other class of comparative group consisting of 16 students. To observe the impacts that applying argumentation activities has on the claim-evidence of the students, writings that the students in the class of experiment group did for 5 argumentation activities were collected, and after the activities, both the experiment group class students and the comparative group class students were assigned to do writings to explain a specific topic. Argument-based inquiry activities were restructured so that CoproC(Collaborative Problem solving for Character competency) is in accordance with the developmental stages of elementary school students, and it was named as 'ALOHOMORAA Program'. ALOHOMORAA Program consists of 6 stages, which are 'Writing Something I Want to Know', 'Planning an Experiment While Loading', 'Solving by Observing with Curiosity', 'Group Discussion and Discuss All Together', 'Looking Back on My Idea' and 'Aha! Explaining the Things I Got to Know'. The writings that the students had done during 'Aha! Explaining the Things I Got to Know' stage, which is the last stage of ALOHOMORAA Program based on CoproC, were analyzed, thus the changes that had occurred upon the claim-evidence along with the progression of the activities were examined.

Poster Presentation : **EDU.P-461**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

The Relationships Between Integrative Creativity and Creativity in Scientific Humor of Elementary Students

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This study investigated the relationships between ‘integrative creativity’ and ‘creativity in scientific humor’ of elementary students. To do this, five graders (n=42) at an elementary school and five graders (n=38) at a gifted science education institutes in Seoul were selected. Tests for ‘integrative creativity’ and ‘creativity in scientific humor’ were then administered. Analysis of the results revealed that the scores for some subcategories of ‘creativity in scientific humor’ were positively correlated with those for ‘integrative creativity’, especially for ‘creative motivation (e.g., curiosity and playfulness)’ and ‘creative potency (e.g., knowledge, imagination, sensitivity, flexibility, and fluency)’ more than ‘creative attitude’. The subcategories of ‘integrated creativity’ that were significantly related to ‘creativity in scientific humor’ were somewhat different according to the subcategories of ‘creativity in scientific humor’. Educational implications of these findings are discussed.

Poster Presentation : **EDU.P-462**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Electrolysis: What Textbooks Don't Tell Us

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We present a critical discussion of how chemistry textbooks treat the electrolysis of water and aqueous salt solutions. Our analysis is based on a survey of general chemistry textbooks in English and Korean at secondary and tertiary levels, also informed by our own experiments and the historical background of 19th-century debates. English-language textbooks present various and contradictory accounts of the electrolysis of water; a key point of disagreement is whether hydrogen and oxygen gases originate from pre-existing H+ and OH- ions, or from the direct reduction and oxidation of H2O molecules. School textbooks in Korea all present the same account, with no indication of alternative views. A vast majority of all texts ignore the possibility that H2 and O2 may result from secondary reactions, which was a standard view in the late 19th century following the works of Daniell and Miller. Concerning the electrolysis of aqueous salt solutions, all of the treatments we have found give oversimplified views of competing reactions based on standard reduction/oxidation potentials. It is understandable that textbooks try to present sufficiently simple pictures that students at each level can handle; however, this should not be done in a way that shuts down questions. We believe that a judicious admission of complexity would be beneficial in encouraging students toward further learning and investigation.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **EDU.P-463**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Writing and Reflecting on the Educational Volunteer Activity in Middle America

JaeYoung Han

Department of Chemistry Education, Chungbuk Natioanl University, Korea

Korean pre-service teachers had gone to a country in middle America, to perform the overseas educational volunteer activity supported by National Institute for International Education. They taught chemistry, physics, biology, mathematics, etc. to the elementary or secondary school students in middle America. After finishing the volunteer activity in Feb. 2019, some pre-service teachers are writing together a book on their experiences of participating the activity. The purpose of this study is to describe the procedure of this work of writing, and to find out what the pre-service teachers have learned in this work. Eight pre-service teachers and one professor have shared the work of writing, such as 'planning,' 'making the list of contents,' 'writing the draft,' 'surveying,' 'commenting,' 'adding,' 'deleting,' 'correcting,' 'editing,' 'proof reading,' etc. The book consists of 10 chapters including, e.g., preparing, role, teaching, co-teacher, etc. The 8 pre-service teachers also made reflections on the process of their co-writing work. They said, for example, that they had an opportunity to share their different thinking on the same volunteer activity, and that they could understand the whole procedure of volunteer activity. The co-writing work gave pre-service teachers another valuable experiences of volunteer activity. [This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2018S1A5A2A01036487)].

Poster Presentation : **EDU.P-464**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Analysis of conceptions and classification results of 10th grade students related to the three states of matter

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In order to examine students' thinking about classification criteria, we required students to establish classification criteria for various cases in everyday life. We also required students to classify the cases based on the classification criteria that they set. We also examined students' classification criteria for the three states of matter and analyzed the results of the classification activities for various substances. In addition, students were asked to clarify the meanings about classification criteria and the procedure for establishing classification criteria. For this study, we conducted a survey for 19 students of 10th grade in Incheon City, and collected the reports of classification activities made by students. The collected data were analyzed by qualitative research method. As a result, the students' classification criteria for the three states of matter remained mainly at the empirical level. In the case of mixtures, the students had difficulty in classifying the state of matter. We found that high school students need educational programs that would allow them to understand the function of the science process of classification.

Poster Presentation : **EDU.P-465**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Analysis of Modeling Ability of 12th grade Science Department Students on Acid and Base Models

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Kongju National University High School, Korea
[1]*Korea National University of Education, Korea*

In this study, we researched that which acid-base models students select in the various contexts and what problems students have during modeling of the acid-base models. For this purpose, 30 students of science department in 12th grade of high school who learned various acid-base models were selected. In order to understand the modeling ability of the students, we developed seven items related to the context of one kind solute and solvent, two kinds solutes and solvent, the case of water solvent, the cases of non-water solvent, etc. As a result, the proportion of students who applied only one model, regardless of context, was 60%. This means that many students do not acquire the ability of modeling in spite of learning science in high school science department. Only 4 (13.3%) out of 30 students understood and responded to the preconditions of the model correctly. 8 students (26.7%) selected various models according to the situation context, but could not select the appropriate model for the problem situation. This implies that students had confused thinking due to lack of understanding of the preconditions of the models. In addition, students frequently showed incomplete modeling while using models. This is because the students did not understand the preconditions of the acid-base models. We suggested that students can not acquire modeling ability if they do not understand and connect with the various prerequisites required in the acid base models. The results showed that students can not acquire modeling ability if they can not understand the various preconditions required in the acid-base models and think about linking the situation context.

Poster Presentation : **EDU.P-466**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Analysis of Problems in the Representation of Acid-Base Model of Chemistry I Textbooks in 2009 Revised Curriculum and 2015 Revised Curriculum

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[1]*Sejong Academy of Science and Art, Korea*
[2]*Kongju National University High School, Korea*

In this study, we analyzed the sub-microscopic representations of the acid-base models presented in the Chemistry Ⅰ textbooks of the 2009 revised curriculum and the 2015 revised curriculum to investigate the causes of students' difficulty in understanding acid-base models. For this purpose, the acid-base contents of nine chemistry Ⅰ textbooks of the 2015 revised curriculum and four chemistry Ⅰ textbooks of the 2009 revised curriculum were analyzed. As a result of analysis, four errors of logical thinking expression and four errors of acid-base model’s precondition were found in the sub-microscopic representation presented in the textbook. These results suggest that it is necessary to present a visualized submicroscopic representation of invisible particles as appropriate for the model. These efforts will help students understand the various acid-base models and concept.

Poster Presentation : **EDU.P-467**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Evaluation of K-MOOC Science Courses Based on Universal Design for Learning Framework

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In this study, K-MOOC (Korean Massive Open Online Courses) science lesson contents and alignments were analyzed in the context of Universal Design for Learning (UDL) which aims barrierless for any type of learners. For UDL Scanning Tool, Korean UDL-Based Instruction Analysis Checklist for Observer was adapted to measure K-MOOC science lessons with three UDL principles nine guidelines and thirty-six checkpoints. One hundred and fifty-eight out of two hundred and ninety-five available K-MOOC science lessons within the content areas of engineering, natural sciences, and medical sciences and pharmacy were randomly selected and evaluated for this study. Result revealed that K-MOOC science lessons were significantly aligned with the UDL principle “provide multiple means of representation” but partially aligned with rest of the two principles e.g. “Provide multiple means of action and expression” and “Provide multiple means of engagement”. While considering the UDL guidelines, the K-MOOC science lessons are significantly aligned with UDL guideline “Provide option for perception” and “Provide options for comprehension.” There were no significant differences among content areas and major facilitating universities.

Poster Presentation : **EDU.P-468**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

Development of Responsive Teaching Capacity through Pre-service teachers' class analysis

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Responsive Teaching is the teacher's ability to draw on students' ideas, interpret them, and lead them to reasoning. Responsive teaching is more of a competence for teachers at this point when student-centered instruction is being emphasized. Robertson et al. (2016) suggest that responsive teaching involves emphasizing the nature of student ideas, finding academic relationships in student ideas, and developing the core of student ideas. Based on these characteristics, we developed and applied the program. Our step-(1) modeling (2) rehearsal (3) Apply (4) Reflection-is based on McDonald et al.(2013) 's training model to improve practical capacity. The study consisted of 14 participants in the Department of Chemistry Education. Their discussion recording, class demonstration recording, class analysis paper, and personal reflection paper were copied and analyzed. This study set up three research questions. First, we develop a responsive teaching analysis framework for pre-service science teachers. Second, based on the analysis of research question 1, it is confirmed how pre-service teachers' change as program proceeds. Third, it explores what is needed in the teacher training program to improve responsive teaching capacity. As a result of the analysis, the pre-service teacher's class analysis was categorized into Design, Listening, Capture, and Turning, and each was divided into two levels. Design refers to the preparation of the teacher's class to elicit the student's ideas, and classified into narrow design and expanded design. Listening was categorized as Superficial and Responsive listening, depending on whether the teacher's response to the elicited student's ideas was accepted as a resource. Capture is searching for possibility of academic linkage to students' ideas identified through listening and classifies them into Selective capture and Interpretive capture. Turning refers to the guidance of a teacher who offers alternatives to verify student ideas identified through listening and capturing. The level of scaffolding behavior is classified into the case of teacher-led and student-led. Ultimately, responsive teaching is a practical competence that is made visible through

turning. In particular, since Turning should be preceded by the interpretation and analysis of student ideas, the future teacher education shows the need for the ability of pre-service teachers to interpret student ideas.

Poster Presentation : **EDU.P-469**

Chemistry Education

Exhibition Hall 1, FRI 11:00~12:30

Introduction of the Korean Translation of the Periodic Table of the Chemical Elements prepared by ACS

Choon Ho Do

Korean Chemical Industry Specialists Association, Korea

Posters describing the Periodic Table of the Chemical Elements were prepared by the American Chemical Society (ACS) in 2018 to celebrate the 150th anniversary of publishing the first periodic table by Mendeleev and International Year of the Periodic Table (IYPT) declared by UN in 2019. The 32 posters contain many fascinating facts, stories and ideas. The English version of the posters by ACS has been translated into many different languages worldwide. We like to introduce the posters translated in Korean.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **EDU.P-470**
Chemistry Education
Exhibition Hall 1, FRI 11:00~12:30

The characteristics on the chemistry students in the science high school: comparative analysis between the mathematics/science achievement and individual differences.

Dong-Seon Shin, Hojune Choi[1], Bong Gon Kim[1,*]

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Science high schools were established at the national level to foster competent engineers/scientists to enhance international competitiveness in science and technology. Recently, the goal of science education has emphasized the development of creative thinking, problem solving ability and convergent thinking ability. It is emphasized without exception in science high school, a special purpose high school. Therefore, the study of science high school students' perception of mathematics/science is a very meaningful task. Therefore, the purpose of this study is to investigate the characteristics of subjects through the method of factor analysis of academic achievement in mathematics and science, and to identify the status of chemistry subjects in students' perceptions. In addition, we tried to analyze the individual differences of chemistry R&E students.This study was conducted with 337 students from three science high schools in Ulsan and Gyeongnam. The individual differences of students used the Sternberg thinking form and the Kolb learning form questionnaire.In the results of this study, the first two factors of mathematics and science achievement of science high school students were classified into two factors: mathematical logic (math and physics) and natural understanding(life science and earth science). Chemistry has been identified as a middle ground between mathematical logic and natural understanding. Second, students with clear mathematical logic factors recognized chemistry as a natural understanding domain, while students with natural clear domain factors recognized chemistry as a mathematical logic domain. Third, the students' academic achievement was well correlated with the Kolb learning style based on the thinking style and information processing theory.

Poster Presentation : **ENVR.P-451**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Aqueous plutonium chemistry and thermodynamics at reducing and elevated temperature conditions

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Plutonium chemistry in aqueous solutions at reducing and elevated temperature conditions should be understood for safety assessment of high-level radioactive waste disposal in deep underground repository. Near-field environments of a proposed repository system are expected to have a reducing and high temperature environment owing to the oxidation of iron and the decay heat of radioactive materials. Aqueous plutonium chemistry (redox-reaction, solubility, hydrolysis, colloid formation, etc.) related to the mobility of Pu in a geological environment (anaerobic, neutral pH, etc.) has been widely investigated [1]. However, experimental investigations on the plutonium hydrolysis and solubility of plutonium hydroxide at elevated temperature are scarce [2]. The aim of this work is the chemical speciation of plutonium hydrolysis species and solubility measurement at different temperatures. The absorption spectra of dilute plutonium samples are measured using a spectrophotometer (Cary5000, Agilent Tech) coupled with a liquid waveguide capillary cell (LWCC) [3] modified for measurements at elevated temperature. The formation of plutonium colloids was observed through laser-induced breakdown detection (LIBD). The typical absorption spectra of Pu^{3+} ions in visible wavelength ranges were not changed with formation of hydrolysis species of Pu(III) at 25 °C [3]. The solubility limit of plutonium hydroxide was determined from the initial colloid formation in solutions. The preliminary results on the study of the hydrolysis of Pu(III) and solubility of plutonium hydroxides at reducing and elevated temperatures will be presented.**References**[1] A. B. Kersting, Inorg. Chem. 52, 3533 (2013).[2] R. Guillaumont, T. Fanghanel, V. Neck, J. Fuger, D. A. Palmer, I. Grenthe, M. H. Rand, “Chemical thermodynamics of uranium, neptunium, plutonium, americium and technetium”, pp. 313-388, Elsevier, North-Holland, Amsterdam (2003). [3] H.-R. Cho, Dalton Trans. 45, 19449 (2016).

Poster Presentation : **ENVR.P-452**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Assessment of mercury bioavailability in Hyeongsan River deposits for earthworm *Eisenia Fetida* using diffusive gradient in thin films technique

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Hyeongsan River has been highly contaminated with Hg discharged from the industrial complexes in Pohang, Korea. In this study, we used diffusive gradient in thin films technique (DGT) and earthworm, *Eisenia Fetida*, to estimate soil Hg bioavailability in relation to the conventional properties, such as, cation exchange capacity (CEC), soil organic matter (SOM), pH, redox potential (ORP), and water holding capacity (WHC), of the soils collected from Hyeongsan River deposits. The Hg concentration in Hyeongsan River soils ranged from 326 to 173,000 ng g^{-1} (I-geo = -0.46 – 8.59) while that in control soils ranged from 10.1 and 10.5 (ng g^{-1}) (I-geo = -5.47 – -4.83). The DGT-Hg flux was found to be highly correlated with Hg in earthworm ($r^2 = 0.80$). The principal component analysis (PCA) was applied to extract information on critical soil properties affecting biota-sediment accumulation factor (BSAF) of Hg. The results revealed that the soil distribution of CEC, ORP, and WHC were commonly linked to SOM, a major factor controlling Hg bioavailability. Moreover, BSAF and DGT-sediment accumulation factor (DSAF) were simulated with partial least square regression (PLSR) model using the soil properties. The PLSR results showed that CEC (VIP = 1.3) and SOM (VIP=1.2) are the most sensitive parameters affecting the BSAF and DSAF of Hg. Overall, we demonstrate that DGT is a useful tool for Hg bioavailability prediction in diverse soils, and the CEC and SOM play the most crucial role in the process of Hg accumulation in earthworm and DGT.

Poster Presentation : **ENVR.P-453**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Porous magnetoelectric films of cobalt ferrite/polyvinylidene fluoride for effective fine dust removal

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Magnetoelectric (ME) effect is a unique material characteristic of induced electrical polarization given by applying magnetic field. In recently, non-contact surface charge induction in ME system was reported for an effective targeting of cancer tumor as a novel drug delivery system.Particulate matter (PM) pollution has a negative impact on human health, climate, and ecosystems. Recently, with serious considerations, many researchers have attempted to filter out the fine dust by controlling filter structure and membrane pore size. But there should be a high-pressure drop reducing breathability and filter efficiency, simultaneously. Thererfore, functional membranes have been developed for an effective dust filteration with minimum pressure-drop by using electrical system or piezoelectric materials. However, there are also critical problems of continuous electric power consumption and space limitation. In this study, we designed a new filter system based on the non-contact surface charge induction from magnetoelectric composite films including magnetostrictive particles of $CoFe_2O_4$ (CFO) and piezoelectric polymers of poly(vinylidene fluoride) (PVDF). First, the CFO nanoparticles were hydrothermally synthesized with a primary particle size of 30 nm. Then porous CFO/PVDF ME films were fabricated via electrospinning process. To optimize surface charge of ME filter memberane for effective capturing of the fine dust, electrospinning conditions were adjusted with respect to CFO variations. As a result, PM removal efficiency was found to be above 99.90% confirmed by particle counter measurement, and pressure drop reduced to 45Pa compare to 500Pa from commercial HEPA filter. Coverage of CFO/PVDF films was about 20cm x 20cm and average pore size of membrane was 15 µm.

Poster Presentation : **ENVR.P-454**

Environmental Energy

Exhibition Hall 1, THU 11:00~12:30

Arsenite oxidation by FeOOH polymorphs

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Arsenic contamination is an enormous worldwide problem. Arsenic exists mainly as arsenite and arsenate in groundwater. It is known that arsenite is harder to be removed than arsenate. So, it is necessary to oxidize the arsenite to arsenate prior to other treatment processes. Electrochemical catalysis has been actively researched as a key technology for oxidation of arsenite. FeOOH polymorphs have important application in electrocatalysis. This study attempted to oxidation of groundwater arsenite using electrocatalyst. FeOOH polymorphs were deposited by chemical bath deposition, hydrothermal deposition and electrodeposition. Arsenite spiked in groundwater was electrochemically oxidized using electrocatalyst FeOOH polymorphs. The physical and chemical properties of FeOOH polymorphs are different. The optimum applied voltage range was 1.1(V. vs SCE) in 0.1M bicarbonate. Lepidocrocite (γ-FeOOH) has highest arsenite oxidation at 1.1(V. vs SCE) in 0.1M bicarbonate without CO2. After reaction for 2hours, Arsenite was oxidized about 30%. This research was supported by the Basic Science Research Program (2018R1A6A1A03024962 and NRF-2019R1A2C2002602) through the National Research Foundation, Korea. In addition, this work was partly supported by the Korea Ministry of Environment as Waste to Energy-Recycling Human Resource Development Project (YL-WE-17-001)

Poster Presentation : **ENVR.P-455**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Rhenium Sulfite Clusters for Solar Cell Application

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In recent years, there has been increasing interest in photoluminescent octahedral clusters [{M6Q8}L6] (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 [Re6Q8(TBP)5(SO3)] (where Q is Se or S) was synthesized and characterized. The structures were confirmed by chemical analysis and energy-dispersive X-ray spectroscopy methods.

Poster Presentation : **ENVR.P-456**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Highly Efficient Luminescent Solar Concentrator Based on a Nanosized Metal Cluster-Polymer Hybrid

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A new luminescent, highly efficient solar concentrator (LSC) that consisted of nanosized metal-clusters as molecular luminophores encapsulated in poly(methyl methacrylate) (PMMA) waveguide is fabricated by simple solution process. To make a highly emissive, transparent, and robust LSC, organic-inorganic salts such as (dMDAEMA)2[Mo6I14] (where dMDAEMA+ refers organic cation, 2-(methacryloyloxy) ethyl dimethyldodecylammonium) are uniformly incorporated in PMMA. Due to the strong absorption at UV-Vis wavelength up to (~500 nm) and the large Stokes shift to the near infrared (~850 nm) emission, this hybrid luminophore allows zero reabsorption resulting efficient UV-Vis sunlight harvesting with low tint. Si photovoltaic cell with dimensions of 2.0 x 0.3 cm2 is placed at the edge of the LSC plate with dimensions of 2.0 x 2.0 x 0.3 cm3. The highest power conversion efficiency (PCE) 1.74% and transparency ~90% observed in this LSC system are significantly higher than previous known LSC systems. In addition to the high-power conversion efficiency, its chemical robustness and simple solution process in fabrication suggest a promising future direction for the development of a practical LSC system for a transparent building-integrated energy harvesting smart windows.

124th General Meeting of the Korean Chemical Society
October 16(Wed)~18(Fri), 2019, Changwon Convention Center, Changwon, Korea

Poster Presentation : **ENVR.P-457**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Application of As(Ⅲ) Oxidation using Titania and Tungsten Trioxide Composite Catalyst Filters

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This study used TiO_2(T) and WO_2(W) composite embedded inorganic membrance system, which has been applied to the charging system. The role of TiO_2 is photo-generation and WO_2 is photo-charging during pre-irradiation. TW membrane filters were charged under UV or simulated solar light irradiation(AM 1.5) and used a flow-type system that penetrates once at a constant flow rate in dark conditions was used. As a prior study, a TW-embedded filtration membrane successfully demonstrated the reduction of hexavalent chromium (Cr(Ⅵ)). Based on this method, it was applied to oxidation of arsenite(As(Ⅲ)) process. During pre-irradiation with UV or AM 1.5, electrons accumulated in TW were used to produced ROSs(Reactive oxygen species). The As(Ⅲ) oxidation efficiency increased with the ratio of TW each and UV irradiation time. Also, this was influenced by reaction conditions (Air, N_2, O_2). TW-embedded membrane is simple to make and be easily reusable and recharged.This research was supported by the Basic Science Research Program (2018R1A6A1A03024962 and NRF-2019R1A2C2002602) through the National Research Foundation, Korea. In addition, this work was partly supported by the Korea Ministry of Environment as Waste to Energy-Recycling Human Resource Development Project (YL-WE-17-001)

Poster Presentation : **ENVR.P-458**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Dissolved oxygen and nitrate effects on the reduction and removal of divalent mercury by pumice supported nanoscale zero-valent iron

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A series of batch experiments were conducted to identify the effects of dissolved oxygen (DO) and nitrate on the removal and reduction of Hg(II) by pumice supported nanoscale zero-valent iron (p-nZVI) composite. After the adsorption and consecutive reduction of Hg(II) in an anoxic solution, zero-valent iron, and ferrous and ferric irons were found on the surface of the p-nZVI with a chain-like structure; while in the oxic solution, a thick ferric shell was found on the surface of the p-nZVI with collapsed chain structures. In Hg(II) sorption isotherm tests, with 25, 250, 1000, and 2500 nM of Hg(II), the Hg(II) sorption capacity of the p-nZVI was 6.1 mg g-1 in the oxic aqueous solution and 1.5 mg g-1 in the anoxic aqueous solution. While the adsorption of Hg(II) was more favorable in the presence of DO, the headspace Hg(0), as well as dissolved Fe(II), was largely increased in the absence of DO. The removal of Hg(II) in oxic and anoxic suspensions was not affected by nitrate levels ranging from 0.08 to 8 mM. In contrast, Hg(0) concentration in headspace increased with an increase of nitrate, which was related to the enhanced dissolved Fe(II) production. The experimental results of this study suggest that the absence of DO and the presence of nitrate in groundwater could significantly increase Hg(0) in groundwater and adjacent atmosphere during the usual remediation process using relevant nZVI techniques. The effective capture and treatment methods of Hg(0) should be developed for better application of p-nZVI-based technologies.

Poster Presentation : **ENVR.P-459**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Development of magnetically separable Cu catalyst supported by steel slag for p-nitrophenol reduction

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Steel slag (SS), produced from steel plants during the conversion of iron ore to steel products, has been known as one of the largely industrial solid waste in the world. Since it contains high portion of CaO, SS is hardly recycled as cementitious material, thus used as simple aggregate or directly disposed into natural environment. In this study, we newly developed a Cu doped magnetic separable catalyst supported by SS for enhanced catalytic reaction of para-nitrophenol (p-NP). Firstly, we washed out SS up to 5 times by magnetic separation method in SS suspension to remove impurities and obtain high magnetic material (MSS). After the Cu doping (Cu@MSS), p-NP was successfully reduced to p-aminophenol in a few minutes in the presence of $NaBH_4$ solution. A variety surface analysis were carried out to characterize the Cu@MSS. In addition, we investigated the effects of environmental factors on the catalytic p-NP reduction such as Cu loading, $NaBH_4$ concentration, and catalyst concentration. Finally, recycling experiments showed that stability and reusability of Cu@MSS during the 5 times reaction.

Acknowledgements
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Poster Presentation : **ENVR.P-460**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Rational design of Indium-doped TiO_2 modified g-C_3N_4 for improved gas-solid phase CO_2 Photoreduction: Interfacial coupling effect and reaction mechanism

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The In-TiO_2/g-C_3N_4 nanocomposite is an important material in photocatalysis, but little attention has been paid to their interfacial interaction in photocatalytic reaction. Herein, we prepare the In-TiO_2/g-C_3N_4 nanocomposites via a two-step mechanically milling and calcination process. The composite exhibited the highest CO_2 photoreduction activity superior to that of the pure g-C_3N_4 and In-TiO_2 in the UV 365nm and visible light. The results of UV–vis DRS, TRPL and photoelectrochemical measurements demonstrated that In-TiO_2/g-C_3N_4 exhibited more visible light adsorption and faster photo-generated charge transfer. Furthermore, the interfacial electronic structures of In-TiO_2/g-C_3N_4 nanocomposites were thoroughly characterized. According to the XPS results, with the help of a strong built-in electric field presenting in the In-TiO_2/g-C_3N_4 interface, the photo-generated electrons flow to the In-TiO_2 from g-C_3N_4, leading to the highly-efficient electron separation and more CO_2 molecules photo-reduction to CO, CH_4 and C_2H_4. This work explicates the significant role of built-in electric field in CO_2 photoreduction on In-TiO_2/g-C_3N_4 photocatalyst.This research was supported by the Basic Science Research Program (2018R1A6A1A03024962 and NRF-2019R1A2C2002602) through the National Research Foundation, Korea

Poster Presentation : **ENVR.P-461**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Effect of humic acid on TiO_2 photocatalytic activity under visible light illumination by ligand-to-metal charge transfer (LMCT) via surface complex formation

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Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea
[1]*Korea Institute of Science and Technology, Korea*

The diverse applications of TiO_2 can cause its exposure into natural water environment and the natural organic matter (NOM), which ubiquitously exists in natural water and soil will strongly affect behavior of TiO_2 with high potential. It is important to elucidate the environmental implications caused by the reaction of TiO_2 and NOM in aquatic system. This study shows that humic acid (HA) as a representative of NOM affects to photocatalytic activity of TiO_2 under visible light (VL) condition through the ligand-to-metal charge transfer (LMCT) by the formation of surface charge transfer complex. The decomposition of some substrates (such as hexavalent chromate (Cr(VI)), 4-chlorophenol (4-CP)) were clearly enhanced in the system containing both HA and TiO_2 compared to controls (HA only and TiO_2 only), whereas that of dichloroacetate (DCA) was not degraded at all. It confirms that HA affect onto TiO_2 photocatalysis under VL condition and the substrate-specific property is related with the location of the reaction occurred. The current increase of TiO_2/FTO electrode with gradual addition of HA and the decrease of PL intensities of HA with increasing dose of TiO_2 indicates that electrons were transferred from HA to the conduction band of TiO_2. The HA-coated TiO_2 (HA/TiO_2) has a continuous absorption in the visible region extending over 700 nm that is not observed in HA or TiO_2 only. It is assigned to the ligand-to-metal charge transfer (LMCT) transition (HA + TiIV --> HA+ + TiIII) induced by surface charge transfer complexation. Generation of diverse ROS by HA/TiO_2 system under was confirmed and among the ROSs, hydrogen peroxide (H_2O_2) was most significantly observed.References[1] G. Zhnag, G. Kim and W. Choi, "Visible light driven photocatlaysis mediated via ligand-to-metal charge transfer (LMCT): an alternative approach to solar activation of titania", Energy Environ. Sci.,, 7, 954-966 (2014)[2] M. Long, J. Brame, F. Qin, J. Bao, Q. Li, and P Alvarez, “Phosphate Changes Effect of Humic Acids on TiO2 photocatalysis: From Inhibition to Mitigation of Electron-Hole RecombinationAcknowledgementThis work was conducted with the support

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Poster Presentation : **ENVR.P-462**
Environmental Energy
Exhibition Hall 1, THU 11:00~12:30

Anatase-rutile synergistic effect in TiO_2 photocatalysis: an assessment of the water-oxidation and pollutant-degradation mechanism

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Numerous studies have investigated photocatalytic properties of anatase, rutile, and TiO_2 (anatase and rutile) composites; however, the detail mechanistic investigations are limited due to the short lifetime of the photogene rated charge carriers. Herein, In order to reveal the synergistic effect between anatase and rutile phase of TiO_2, the photo-(electrochemical) activity of slurry type and electrode type of two main crystalline were systematically investigated. In particular, the charge transfer process between polymorphs were directly observed using time-resolved diffuse reflectance spectroscopy method. In slurry type, no photocatalytic synergic effect between anatase and rutile was observed while the photo-electrochemical synergic effect was clearly represented in electrode type system, which is consisted with the charge transfer dynamic data from laser flash photolysis. In addition, using FT-IR spectroscopy technique, the recent result of mechanism will be discussed.

Poster Presentation : **ENVR.P-463**

Environmental Energy

Exhibition Hall 1, THU 11:00~12:30

Electrochemical energy storage evaluation of the nanostructured V_2O_5 prepared via one-step anodization

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Recently energy storage has become a big issue since most of the energy devices have either low energy and/or power densities. So it is essential to develop highly capacitive energy storage devices. Among energy storage devices, pseudocapacitive energy storage devices (Supercapacitors) have been attracting great attention because of its intermediate position of energy and power density on the Ragone plot. Several materials are being investigated for enhancement of the energy and power density of the supercapacitors. Among various materials, especially vanadium pentoxide (V_2O_5) is one of the most attractive materials because it has high theoretical capacity due to several oxidation states enabling multiple electron transfer. Various wet chemical methods have been used to prepare V_2O_5, however these methods time consuming, require additional binders to form the electrodes. Herein, we fabricated vertically aligned V_2O_5 nanostructure directly on the vanadium metal substrate by anodization and evaluated electrochemical performances for high energy density electrochemical application.

Poster Presentation : **ENVR.P-464**

Environmental Energy

Exhibition Hall 1, THU 11:00~12:30

Formation behavior of nanoporous oxide films formed by anodization on stainless steel in hot glycerol electrolyte

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Self-organized nanoporous anodic films formed by anodization have various advantages due to its high specific surface areas, high electron conductivity with vertically aligned morphology. For these reasons, anodization has been used in electrodes for energy devices or catalyst supports requiring a large surface area. In general, porous anodic $A_{l2}O_3$ are formed in acidic electrolytes, anodic TiO_2 nanotubes are formed in fluorine containing electrolytes at room temperatures. In this presentation, we fabricated porous Fe_2O_3 films on stainless steel using phosphate containing hot glycerol electrolyte for high efficiency electrolysis electrodes. As a result, we found optimum condition of porous oxide films in various temperatures and applied voltage.